Flow-equation approach to quantum systems driven by an amplitude-modulated time-periodic force

Viktor Novičenko ⬡,* Giedrius Žlabys ⬡,† and Egidijus Anisimovas ⬡‡

Institute of Theoretical Physics and Astronomy, Vilnius University, Saulėtekio Avenue 3, 10257 Vilnius, Lithuania

We apply the method of flow equations to describe quantum systems subject to a time-periodic drive with a time-dependent envelope. The driven Hamiltonian is expressed in terms of its constituent Fourier harmonics with amplitudes that may vary as a function of time. The time evolution of the system is described in terms of the phase-independent effective Hamiltonian and the complementary micromotion operator that are generated by deriving and solving the flow equations. These equations implement the evolution with respect to an auxiliary flow variable and facilitate a gradual transformation of the quasienergy matrix (the Kamiltonian) into a block-diagonal form in the extended space. We construct a flow generator that prevents the appearance of additional Fourier harmonics during the flow, thus enabling implementation of the flow in a computer algebra system. Automated generation of otherwise cumbersome high-frequency expansions (for both the effective Hamiltonian and the micromotion) to an arbitrary order thus becomes straightforward for driven Hamiltonians expressible in terms of a finite algebra of Hermitian operators. We give several specific examples and discuss the possibility to extend the treatment to cover rapid modulation of the envelope.

I. INTRODUCTION

Periodically driven quantum systems [1,2] constitute an immensely practical [3] and at the same time quite tractable intermediate case between the two limits of stationary and generic time-dependent systems. The former limit of systems governed by time-independent Hamiltonians looks much simpler due to the availability of well-developed notions, methods, intuition, and a relatively low numerical complexity. Here the time evolution is readily available in terms of the exponentiated Hamiltonian. In contrast, the evolution of a generic time-dependent system is described by the time-ordered exponential of a Hamiltonian operator that does not commute with itself at different instants of time. The evolution operator may be simple to write down, but its evaluation for a nontrivial system requires considerable effort [4–6].

The theoretical description of periodically driven quantum systems, the Floquet theory [1,2,7–9], is by now well established and forms the basis of Floquet engineering [3,10–18] that is related to numerous experimental highlights [3,15,19–25] (see also Refs. [26–31]). The time evolution of a periodically driven system can be separated into the long-term dynamics governed by a time-independent effective Hamiltonian and micromotion that literally captures the periodic micromotion in the course of a single period of the drive [2,14,15,32–34]. We emphasize from the outset that two distinct approaches to the formulation of the effective Hamiltonian are possible [3,14]. In our paper, as well as in many other works [32–34], we will aim to derive a long-term Hamiltonian that not only is stationary, but also does not

depend on the phase of the drive. We reserve the term *Floquet effective* Hamiltonian to refer to this particular case. In an alternative approach, one uses a long-term Hamiltonian that is more appropriately called the *Floquet stroboscopic* Hamiltonian (or just the Floquet Hamiltonian [3]). The Floquet stroboscopic Hamiltonian [2,9,14,35,36] is straightforwardly defined as the logarithm of the evolution operator over a single period of the drive and is perfectly suited to describe the evolution between two instants of time separated by an integer multiple of the period. Note, however, that there exists a whole family of such Hamiltonians, parametrized by the phase of the drive or, equivalently, by the initial time.

Systematic construction of Floquet Hamiltonians has been achieved through a number of approaches [33,34,37–39], for example, various formulations of the perturbation theory, transition to the extended space, and unitary flows towards diagonalization (or block diagonalization) defined by a sequence of elemental transformations. In many cases, the Floquet effective Hamiltonian is constructed order by order as an expansion in powers of the inverse frequency of the drive [14,33,34,38,40]. Importantly, such expansions support a transparent physical interpretation of the generated terms, which is a crucial asset in devising synthetic quantum systems that mimic various phenomena of condensed-matter physics [2,3,15,34]. For open systems, work on extension to Floquet Lindbladians has begun [41–46].

An important extension is related to the inclusion of an additional temporal modulation of the envelope of the driving signal [40,47–49]. On the one hand, this situation is very practical since it describes a whole class of experimentally relevant setups involving transient signals [48,50]. On the other hand, although technically the drive is not periodic, it fits well into the described scheme of systematic construction of effective Hamiltonians: The high-frequency (or alternative) expansions are typically formulated in terms of Fourier

components of the driven Hamiltonian and it appears conceptually straightforward to endow these components with an additional argument of slow time, thus describing the modulation of the envelope. Proceeding along this line of thought, the authors of Ref. [40] obtained expressions of the effective Hamiltonian and the micromotion to second order in the inverse frequency. They were able to give a compelling example characterized by a non-Abelian geometric phase [51] that emerges precisely from the presence of the time derivative of the Fourier component. In another development, a situation relevant to fast coherent manipulation of a qubit was treated [48,49]. There the authors focused on the accurate stroboscopic description and, employing the Magnus-Taylor expansion, were able to proceed to high orders featuring combinations of the time derivatives of the Fourier components.

The purpose of the present paper is to explore the field of amplitude-modulated periodically driven Hamiltonians relying on the idea of unitary flows [39,52–57]. Originally introduced to eliminate unwanted couplings in many-body problems [52,58], these flows draw inspiration from the renormalization semigroup [59,60] and feature a sequence of elemental (infinitesimal in continuous flows or finite in discrete flows) unitary transformations that make the Hamiltonian gradually morph from the original form to the desired final form, in our case, the block-diagonal form in the extended space. We set out to systematically construct both the effective Hamiltonian and the micromotion operator. As the formulation of the flow is notably nonunique, we develop and use a specific variant, called the Toda flow, that avoids proliferation of constituent Fourier components. When the Hamiltonian can furthermore be expressed in terms of a finite number of Hermitian (Lie) generators, the flow equations are perfectly suited for an automated treatment with the aid of computer algebra systems. We have implemented such a general-purpose procedure to derive the high-frequency expansion to an arbitrary order and describe several paradigmatic examples.

Our paper has the following structure. In Sec. II we introduce the essential notions and tools used in the description of periodically driven systems. In Sec. III we review the idea of unitary flows towards diagonalization and generalize this tool to the block diagonalization of the extended-space quasienergy operator (also known as the Kamiltonian) in Sec. IV. Proceeding to applications, in Sec. V we consider the automated high-frequency expansion and describe several examples in Sec. VII. Section VI is devoted to attempts to go beyond the slow modulation of the envelope. A number of technical issues, such as derivation of equations and proofs, are relegated to the Appendixes.

II. FLOQUET HAMILTONIAN: STROBOSCOPIC VS EFFECTIVE

A. Floquet stroboscopic Hamiltonian

Let us consider a quantum system described by a time-periodic Hamilton operator $h(\omega t + 2\pi) = h(\omega t)$ and obeying the time-dependent Schrödinger equation

$$i\hbar \frac{d|\psi(t)\rangle}{dt} = h(\omega t)|\psi(t)\rangle. \tag{1}$$

The time-evolution operator $U(t_{\text{fn}}, t_{\text{in}})$, which defines the unitary evolution of the state vector $|\psi(t_{\text{fn}})\rangle = U(t_{\text{fn}}, t_{\text{in}})|\psi(t_{\text{in}})\rangle$ from the initial time instant t_{in} to the final time t_{fn}, can be formally written in terms of $h(\omega t)$ as a time-ordered exponential

$$U(t_{\text{fn}}, t_{\text{in}}) = \mathcal{T} \exp\left[-\frac{i}{\hbar} \int_{t_{\text{in}}}^{t_{\text{fn}}} h(\omega t)dt\right]. \tag{2}$$

If the duration of the time interval is an exact multiple of the period of the drive $T = 2\pi/\omega$, that is, $t_{\text{fn}} - t_{\text{in}} = NT$, the periodicity of the Hamilton operator ensures that the full evolution fulfills $U(t_{\text{fn}}, t_{\text{in}}) = [U(t_{\text{in}} + T, t_{\text{in}})]^N$. It is thus natural to introduce the Floquet stroboscopic (FS) Hamiltonian defined as the logarithm of the stroboscopic evolution operator

$$U(t_{\text{in}} + T, t_{\text{in}}) = \mathcal{T} \exp\left[-\frac{i}{\hbar} \int_{t_{\text{in}}}^{t_{\text{in}}+T} h(\omega t)dt\right]$$

$$= \exp\left[-\frac{i}{\hbar} h_{\text{FS}}(t_{\text{in}})T\right]. \tag{3}$$

We note that the FS Hamiltonian $h_{\text{FS}}(t_{\text{in}} + T) = h_{\text{FS}}(t_{\text{in}})$, albeit stationary, periodically depends on the initial time or, equivalently, on the phase of the drive in a parametric way. Thus, when the initial phase is not fixed, one needs to deal with all possible initial phases, that is, with a whole family of FS Hamiltonians. Another downside of the FS Hamiltonian is that it is unambiguously defined only for systems driven in a purely periodic way. In specific cases it was extended to incorporate a modulation of the envelope by introducing a custom-made definition [47,48]. The general redefinition of the FS Hamiltonian for modulated systems is not available.

Equation (3) gives a definition, but does not yet provide a recipe for how the FS Hamiltonian can be found analytically. For an arbitrary Hamiltonian $h(\omega t)$, an exact analytical expression of h_{FS} cannot be found; thus approximate methods are applicable. One of the well-established methods relies on the series expansion in powers of the inverse frequency of the drive. If matrix elements $h_{ij}(t) = \langle\psi_i|h(\omega t)|\psi_j\rangle$ are smaller than the characteristic energy of the periodic drive $\hbar\omega$, one can apply the Magnus expansion [61,62] to the unitary evolution featured in Eq. (3) to obtain the high-frequency expansion $h_{\text{FS}} = h_{\text{FS}(0)} + h_{\text{FS}(1)} + h_{\text{FS}(2)} + O(\omega^{-3})$, with

$$h_{\text{FS}(0)} = \frac{1}{2\pi} \int_{\theta_{\text{in}}}^{\theta_{\text{in}}+2\pi} h(\theta)d\theta, \tag{4a}$$

$$h_{\text{FS}(1)} = \frac{1}{2(i\hbar\omega)} \frac{1}{2\pi} \int_{\theta_{\text{in}}}^{\theta_{\text{in}}+2\pi} \int_{\theta_{\text{in}}}^{\theta_1} [h(\theta_1), h(\theta_2)]d\theta_2 d\theta_1, \tag{4b}$$

$$h_{\text{FS}(2)} = \frac{1}{6(i\hbar\omega)^2} \frac{1}{2\pi} \int_{\theta_{\text{in}}}^{\theta_{\text{in}}+2\pi} \int_{\theta_{\text{in}}}^{\theta_1} \int_{\theta_{\text{in}}}^{\theta_2} \{[h(\theta_1), [h(\theta_2), h(\theta_3)]]$$
$$+ [h(\theta_3), [h(\theta_2), h(\theta_1)]]\}d\theta_3 d\theta_2 d\theta_1, \tag{4c}$$

where $\theta_{\text{in}} = \omega t_{\text{in}}$ is the initial phase. Further terms of the Magnus expansion can be constructed recursively [62].

A different method to obtain the FS Hamiltonian employs a continuous flow of unitary transformations that gradually transform the time-periodic $h(\omega t)$ into the stationary h_{FS} [39]. This approach involves solving the flow equation, which typically cannot be done analytically as well. Instead, the flow equation is used as a starting point for further approximations.

In this paper we present a similar flow approach, formulated not for the FS Hamiltonian but for a phase-independent Floquet effective Hamiltonian that also includes the effects of a time-dependent drive envelope.

B. Floquet effective Hamiltonian

To proceed, let us consider a quantum system described by the Hamiltonian $h(\omega t, t)$, which is a 2π-periodic function of the first argument and also allows for an additional modulation of the envelope through the dependence on time in the second argument. Following Refs. [40,63], we will study the whole family of solutions $|\psi_\theta(t)\rangle$, where $\theta \in [0, 2\pi)$ represents the initial phase. The Hamiltonian $h(\omega t + \theta, t)$ thus also becomes dependent on the initial phase. The evolution is governed by the time-dependent Schrödinger equation

$$i\hbar \frac{d|\psi_\theta(t)\rangle}{dt} = h(\omega t + \theta, t)|\psi_\theta(t)\rangle \qquad (5)$$

and the initial condition at t_{in} is assumed to be θ periodic, i.e., $|\psi_{\theta+2\pi}(t_{\text{in}})\rangle = |\psi_\theta(t_{\text{in}})\rangle$. Thus, it remains periodic throughout the evolution and can be expanded in a Fourier series as

$$|\psi_\theta(t)\rangle = \sum_{n=-\infty}^{+\infty} e^{in\theta}|\psi^{(n)}(t)\rangle. \qquad (6)$$

The corresponding expansion of the Hamiltonian reads

$$h(\omega t + \theta, t) = \sum_{n=-\infty}^{+\infty} e^{in(\omega t + \theta)}h^{(n)}(t), \qquad (7)$$

with $[h^{(n)}(t)]^\dagger = h^{(-n)}(t)$ imposed by Hermiticity. Note that the Fourier components $h^{(n)}(t)$ are time dependent as a consequence of the second argument in the initial Hamiltonian, $h(\omega t + \theta, t)$.

The state vector $|\psi_\theta(t)\rangle$ parametrically depends on θ and is assumed to belong to a physical Hilbert space $\mathscr{H}$. Our next step is to introduce an extended vector space and reformulate Eq. (5) in a new formalism. The idea to introduce the extended vector space for purely time-periodic quantum systems first appeared in Ref. [8]. Because of the θ periodicity, it is natural to introduce the space $\mathscr{T}$ of square-integrable functions periodic on the interval $[0, 2\pi)$. The exponents $e^{in\theta}$ with $n \in \mathbb{Z}$ form the standard orthonormal basis $|n\rangle$ with a dot product defined as $\langle m|n\rangle = (2\pi)^{-1}\int_{-\pi}^{\pi} e^{-im\theta}e^{in\theta}d\theta = \delta_{mn}$. Now one can build the extended space $\mathscr{L} = \mathscr{T} \otimes \mathscr{H}$ as the tensor product of the physical space and the space of θ-periodic functions. The state vector in Eq. (6) can be interpreted as a time-dependent vector (we will use double bra-ket notation for the vectors in the extended space and calligraphic letters for operators acting in the extended space)

$$|\psi(t)\rangle\rangle = \sum_{n=-\infty}^{+\infty} |n\rangle \otimes |\psi^{(n)}(t)\rangle \qquad (8)$$

belonging to the space $\mathscr{L}$ where θ is no longer a parameter but an intrinsic variable of the space. The Hamiltonian (7) can also be interpreted as an operator acting in $\mathscr{L}$:

$$\mathcal{H}(\omega t, t) = \sum_{n,m=-\infty}^{+\infty} |n+m\rangle e^{in\omega t}\langle m| \otimes h^{(n)}(t). \qquad (9)$$

However, the above procedure does not yet simplify the analysis as the operator (9) still contains the time-periodic argument ωt. To eliminate this dependence, one applies the time-dependent unitary transformation

$$\mathcal{U} = e^{\omega t(d/d\theta)} = \sum_{n=-\infty}^{+\infty} |n\rangle e^{in\omega t}\langle n| \otimes \mathbf{1}_{\mathscr{H}} \qquad (10)$$

to Eq. (5), which should be interpreted in the extended space. From Eq. (10) one can see that the unitary transformation shifts the phase variable: $\mathcal{U}^\dagger \theta \mathcal{U} = \theta - \omega t$. Therefore, the argument $\omega t + \theta$ simplifies to just θ. The transformed state vector $|\phi(t)\rangle\rangle = \mathcal{U}^\dagger|\psi(t)\rangle\rangle$ obeys the time-dependent Schrödinger equation

$$i\hbar \frac{d|\phi(t)\rangle\rangle}{dt} = \mathcal{K}(t)|\phi(t)\rangle\rangle, \qquad (11)$$

with

$$\mathcal{K}(t) = \mathcal{U}^\dagger \mathcal{H}(\omega t, t)\mathcal{U} - i\hbar \mathcal{U}^\dagger \frac{d\mathcal{U}}{dt}, \qquad (12)$$

which is often referred to as the Kamiltonian. In the differential form, the obtained Kamiltonian reads

$$\mathcal{K}(t) = -i\hbar\omega \frac{d}{d\theta} \otimes \mathbf{1}_{\mathscr{H}} + \sum_{n=-\infty}^{+\infty} e^{in\theta} \otimes h^{(n)}(t), \qquad (13)$$

while in the bra-ket notation it reads

$$\mathcal{K}(t) = \sum_{n=-\infty}^{+\infty} |n\rangle n\hbar\omega\langle n| \otimes \mathbf{1}_{\mathscr{H}}$$
$$+ \sum_{n,m=-\infty}^{+\infty} |m\rangle\langle n| \otimes h^{(m-n)}(t). \qquad (14)$$

From Eqs. (13) and (14) one can see that the Kamiltonian does not contain the time-periodic argument ωt and depends on time only through the second argument in the original Hamiltonian, $h(\omega t, t)$. If the original Hamiltonian is purely periodic, the Kamiltonian becomes time independent and one can rely on methods developed for time-independent operators, e.g., various formulations of the perturbation theory. However, this comes at the cost of working in the extended space $\mathscr{L}$, while the original problem was formulated in the simpler physical space $\mathscr{H}$.

The Kamiltonian $\mathcal{K}(t)$ can be represented as an infinite matrix where the matrix elements $K_{mn}(t) = \langle m|\mathcal{K}(t)|n\rangle$ are operators in $\mathscr{H}$. Such a matrix possesses some obvious symmetries; for example, the first upper diagonal is filled with copies of the same operator $K_{n,n+1} = h^{(-1)}(t)$. In order to make this symmetry explicit, we introduce the shift operator $P_m = \sum_n |n+m\rangle\langle n|$ and the number operator $N = \sum_n |n\rangle n\langle n|$ (both acting in $\mathscr{T}$) and rewrite Eq. (14) in terms of these operators

$$\mathcal{K}(t) = \hbar\omega N \otimes \mathbf{1}_{\mathscr{H}} + \sum_{m=-\infty}^{+\infty} P_m \otimes h^{(m)}(t). \qquad (15)$$

This expression constitutes a concise statement of the problem.

The next step is to block diagonalize the Kamiltonian. More concretely, we assume that there exists a time-dependent

unitary operator $\mathcal{D}(t)$ such that the transformed state vector $|\chi(t)\rangle\!\rangle = \mathcal{D}^{\dagger}|\phi(t)\rangle\!\rangle$ obeys the time-dependent Schrödinger equation

$$i\hbar\frac{d|\chi(t)\rangle\!\rangle}{dt} = \mathcal{K}_{D}(t)|\chi(t)\rangle\!\rangle, \qquad (16)$$

with the block-diagonal Kamiltonian

$$\mathcal{K}_{D}(t) = \mathcal{D}^{\dagger}\mathcal{K}(t)\mathcal{D} - i\hbar\mathcal{D}^{\dagger}\frac{d\mathcal{D}}{dt}$$
$$= \hbar\omega N \otimes \mathbf{1}_{\mathscr{H}} + P_{0} \otimes h_{\text{eff}}(t). \qquad (17)$$

The operator $h_{\text{eff}}(t)$ is the Floquet effective (FE) Hamiltonian [32–34] acting in the physical space $\mathscr{H}$. Crucially, $h_{\text{eff}}(t)$ does not depend on the initial phase. Indeed, we start from $h(\omega t + \theta, t)$, which depends on the initial phase θ and arrive at the θ-independent $h_{\text{eff}}(t)$.

The block-diagonalization procedure and symmetries allow us to restrict the analysis to the zeroth Floquet subspace $\mathscr{L}_{0}$ spanned by the vectors $|0\rangle \otimes |\psi_{i}\rangle$, where $|\psi_{i}\rangle$ are the basis vectors of the physical space $\mathscr{H}$ and $i \in \{1, 2, \ldots, \dim[\mathscr{H}]\}$. Thus the subspace $\mathscr{L}_{0}$ is isomorphic to the physical space $\mathscr{H}$. The solutions for other Floquet subspaces $\mathscr{L}_{n}$ with $n \neq 0$ can be easily recovered from the solution in the subspace $\mathscr{L}_{0}$. Indeed, let us assume that at the initial time the state vector in Eq. (16) reads $|\chi(t_{\text{in}})\rangle\!\rangle = \sum_{n=-\infty}^{+\infty} |n\rangle \otimes |\chi_{n}(t_{\text{in}})\rangle$. Then Eq. (16) decouples into copies of the Schrödinger equation defined in the subspaces $\mathscr{L}_{n}$ as

$$i\hbar\frac{d|\chi_{n}(t)\rangle}{dt} = [n\hbar\omega + h_{\text{eff}}(t)]|\chi_{n}(t)\rangle. \qquad (18)$$

By defining the evolution operator of Eq. (18) for $n = 0$ as a time-ordered exponential

$$U_{\text{eff}}(t_{\text{fn}}, t_{\text{in}}) = \mathcal{T}\exp\left[-\frac{i}{\hbar}\int_{t_{\text{in}}}^{t_{\text{fn}}} h_{\text{eff}}(t)dt\right], \qquad (19)$$

one can write the full evolution of Eq. (16) as

$$|\chi(t_{\text{fn}})\rangle\!\rangle = \mathcal{U}_{\text{eff}}(t_{\text{fn}}, t_{\text{in}})|\chi(t_{\text{in}})\rangle\!\rangle$$
$$= \sum_{n=-\infty}^{+\infty} e^{-in\omega(t_{\text{fn}}-t_{\text{in}})}|n\rangle \otimes U_{\text{eff}}(t_{\text{fn}}, t_{\text{in}})|\chi_{n}(t_{\text{in}})\rangle. \qquad (20)$$

The Kamiltonians before the block diagonalization $\mathcal{K}(t)$ and after the block diagonalization $\mathcal{K}_{D}(t)$ possess the same symmetry, allowing them to be written in terms of the shift operator P_{m} and the number operator N. This implies [40] that the unitary operator $\mathcal{D}(t)$ can be written as $\mathcal{D}(t) = \sum_{m=-\infty}^{+\infty} P_{m} \otimes D^{(m)}(t)$, and because of unitarity, the operators $D^{(m)}(t)$ satisfy

$$\sum_{m=-\infty}^{+\infty} [D^{(m)}(t)]^{\dagger}D^{(m+l)}(t) = \delta_{0l}\mathbf{1}_{\mathscr{H}}. \qquad (21)$$

Let us recall that starting from the state vector $|\psi_{\theta}(t)\rangle$ in the physical space $\mathscr{H}$, we reformulated the task in the extended space $\mathscr{L}$ for the state vector $|\psi(t)\rangle\!\rangle$, then performed the unitary transformation (10) to obtain the state vector $|\phi(t)\rangle\!\rangle$, and subsequently applied the unitary transformation $\mathcal{D}(t)$ to arrive at the state vector $|\chi(t)\rangle\!\rangle$, for which we are able to write the

solution (20). The full evolution in the extended space reads

$$|\psi(t_{\text{fn}})\rangle\!\rangle = \mathcal{U}(t_{\text{fn}})\mathcal{D}(t_{\text{fn}})\mathcal{U}_{\text{eff}}(t_{\text{fn}}, t_{\text{in}})\mathcal{D}^{\dagger}(t_{\text{in}})\mathcal{U}^{\dagger}(t_{\text{in}})|\psi(t_{\text{in}})\rangle\!\rangle. \qquad (22)$$

However, one needs to transform back to the physical space. In order to write the solution in the physical space, for simplicity, let us assume that at the initial time moment $|\psi_{\theta}(t_{\text{in}})\rangle$ has only the zeroth Fourier component $|\psi_{\theta}(t_{\text{in}})\rangle = |\psi^{(0)}(t_{\text{in}})\rangle$. This means that, analyzing the θ-dependent family of solutions, we have the same initial state vector $|\psi^{(0)}(t_{\text{in}})\rangle$ for all θ. Substituting such an initial state vector into Eq. (22) gives

$$|\psi(t_{\text{fn}})\rangle\!\rangle = \sum_{m,n=-\infty}^{+\infty} |n-m\rangle \otimes [D^{(n)}(t_{\text{fn}})e^{in\omega t_{\text{fn}}}]$$
$$\times U_{\text{eff}}(t_{\text{fn}}, t_{\text{in}})[D^{(m)}(t_{\text{in}})e^{im\omega t_{\text{in}}}]^{\dagger}|\psi^{(0)}(t_{\text{in}})\rangle. \qquad (23)$$

Translating the ket $|n-m\rangle$ into the corresponding exponent $e^{i(n-m)\theta}$, this expression can be interpreted as a vector in the physical space which parametrically depends on θ,

$$|\psi_{\theta}(t_{\text{fn}})\rangle = U_{\text{micro}}(\omega t_{\text{fn}} + \theta, t_{\text{fn}})U_{\text{eff}}(t_{\text{fn}}, t_{\text{in}})$$
$$\times U_{\text{micro}}^{\dagger}(\omega t_{\text{in}} + \theta, t_{\text{in}})|\psi^{(0)}(t_{\text{in}})\rangle, \qquad (24)$$

where the unitary operator

$$U_{\text{micro}}(\omega t + \theta, t) = \sum_{n=-\infty}^{+\infty} D^{(n)}(t)e^{in(\omega t + \theta)} \qquad (25)$$

is called the micromotion operator. The unitarity of Eq. (25) follows from Eq. (21). The motivation behind such a name reflects the fact that it represents deviations from the effective evolution governed by $h_{\text{eff}}(t)$. Importantly, the micromotion depends on the initial phase θ and is applied only at the initial and the final time moments, while the effective evolution is θ independent but applies throughout the time interval. Note that the unitary operator $\mathcal{D}(t)$ and $h_{\text{eff}}(t)$ are not easy to find. We will construct their explicit expressions in the high-frequency regime, i.e., by analyzing the high-frequency expansions of the flow equations.

C. A subtlety

Let us now discuss a special case of a time-dependent perturbation that acts only within a certain time interval fully contained between the initial and the final times t_{in} and t_{fn}, respectively, within the observed evolution. In other words, the Hamiltonian at the initial and the final time instants is stationary $h(\omega t_{\text{in}} + \theta, t_{\text{in}}) = h(\omega t_{\text{fn}} + \theta, t_{\text{fn}}) = h_{0}$; however, at intermediate times, as the perturbation is gradually turned on and subsequently off, the Hamiltonian is characterized by a periodic time dependence with a time-dependent envelope. Since the operator $\mathcal{D}(t)$ seeks to block diagonalize the Kamiltonian (15) and by construction $\mathcal{K}(t_{\text{in}}) = \mathcal{K}(t_{\text{fn}})$ is already block diagonal, one may be tempted to assume that $\mathcal{D}(t_{\text{in}}) = \mathcal{D}(t_{\text{fn}}) = \mathbf{1}_{\mathscr{L}}$ and thus the micromotion operator at t_{in} and t_{fn} is equal to the unit operator. This however leads to an obvious contradiction: If $\mathcal{D}(t_{\text{in}}) = \mathcal{D}(t_{\text{fn}}) = \mathbf{1}_{\mathscr{L}}$, then according to Eq. (24) the final state does not depend on the initial phase θ, while the shape of the perturbation in general depends on θ. This contradiction can be resolved by analyzing the equation for $\mathcal{D}(t)$. Let us say that the FE Hamiltonian

$h_{\text{eff}}(t)$ is known from a different source [not from Eq. (17)]; then from Eq. (17) one can write

$$i\hbar \frac{d\mathcal{D}}{dt} = \mathcal{K}\mathcal{D} - \mathcal{D}\mathcal{K}_D. \qquad (26)$$

Having solved the differential Eq. (26) with the initial condition $\mathcal{D}(t_{\text{in}}) = \mathbf{1}_{\mathscr{L}}$, we will obtain a particular $\mathcal{D}(t_{\text{fn}}) \neq \mathbf{1}_{\mathscr{L}}$ which will not be of the block-diagonal form, featuring nonzero $D^{(n)}(t_{\text{fn}})$ for $n \neq 0$, and moreover will be time dependent, meaning that $\mathcal{D}(t_{\text{fn}} - dt) \neq \mathcal{D}(t_{\text{fn}})$ for an infinitesimal dt. However, $\mathcal{D}(t_{\text{fn}})$ will still be able to block diagonalize the Kamiltonian: After application of Eq. (17) to the block-diagonal operator $\mathcal{K}(t_{\text{fn}})$, the transformed operator $\mathcal{K}_D(t_{\text{fn}})$ will be also block diagonal. Because of such features of the operator $\mathcal{D}(t_{\text{fn}})$, the micromotion $U_{\text{micro}}(\omega t_{\text{fn}} + \theta, t_{\text{fn}})$ will become θ dependent, which resolves the contradiction. In fact, this is an open question: When is it possible to find such $h_{\text{eff}}(t)$ that both $\mathcal{D}(t_{\text{in}})$ and $\mathcal{D}(t_{\text{fn}})$ will have a block-diagonal form [note that if $\mathcal{D}(t)$ has the block-diagonal form $\mathcal{D}(t) = P_0 \otimes D^{(0)}(t)$, then $U_{\text{micro}}(\omega t + \theta, t) = D^{(0)}(t)$ does not depend on θ]? At least one satisfactory case is when the high-frequency expansion is applicable [40]. From the high-frequency expansion it is intuitively clear that the envelope of the perturbation changes slowly over one period of periodic signal and thus the final state (24) does not depend on the initial phase θ.

D. Summary so far

Let us summarize this rather lengthy section. We distinguish two different approaches to describe a periodically driven quantum system: one based on the Floquet stroboscopic Hamiltonian and another based on the Floquet effective Hamiltonian. The FS Hamiltonian can be defined for purely periodic systems while the FE Hamiltonian is possible to define even when the original Hamiltonian is modulated by a time-dependent envelope. The FS Hamiltonian depends on the initial phase of the periodic perturbation and describes the evolution of the quantum system on a time interval which is an integer multiple of the period. In contrast, the FE Hamiltonian does not depend on the initial phase and gives the evolution of the quantum system on an arbitrary time interval. In principle, both Hamiltonians can be used to describe the evolution over arbitrary time intervals: The effective evolution should be sandwiched by the micromotion operators, which in general depend on the initial phase, whereas the stroboscopic description also comes with its own version of phase-dependent micromotion [2]. The FE Hamiltonian is most useful when the micromotion operator does not depend on the initial phase, for example, in the high-frequency limit, when the periodic perturbation with a slowly modulated amplitude does not act at the beginning and at the end of the time interval. Both Hamiltonians (FS and FE) are well defined but difficult to find analytically for an arbitrary frequency; thus one often resorts to a high-frequency expansion. For the FS Hamiltonian the high-frequency expansion implies that ω sets the dominant scale in the sense that any matrix element $h_{ij}(\omega t) = \langle \psi_i | h(\omega t) | \psi_j \rangle$, when expanded into the Fourier series $h_{ij}(\omega t) = \sum_m h_{ij}^{(m)} \exp(im\omega t)$, is characterized by Fourier amplitudes $|h_{ij}^{(m)}|$ that are smaller than the characteristic energy of the periodic drive $\hbar\omega$. For the FE

Hamiltonian the high-frequency expansion additionally assumes that the time-dependent Fourier amplitudes $|h_{ij}^{(m)}(t)|$ only slowly depend on time, $d|h_{ij}^{(m)}(t)|/dt \ll \omega|h_{ij}^{(m)}(t)|$. In such expansion formulas, the FE Hamiltonian reads simpler than the FS Hamiltonian due to the independence on the initial phase, and hereafter we will focus exclusively on the FE Hamiltonian. In Secs. IV B and IV C we derive flow equations that could in principle be used to find the FE Hamiltonian for an arbitrary frequency. Yet the solution of the flow equations is as difficult to obtain as it is to find the unitary operator $\mathcal{D}(t)$ that block diagonalizes the Kamiltonian. Thus Appendixes B and C and Sec. V are devoted to the solution of the flow equations in the form of the high-frequency expansion. Finally, in Sec. VI we perform the high-frequency expansion by relaxing the requirement of the slow time dependence, i.e., the inequality $d|h_{ij}^{(m)}(t)|/dt \ll \omega|h_{ij}^{(m)}(t)|$ is no longer imposed.

III. FLOW TOWARDS DIAGONALIZATION

Originally introduced in the context of many-particle problems [58], flow equations establish a method to gradually bring a Hamiltonian closer to the diagonal form by applying a sequence of specifically tailored unitary transformations. In practice, a time-independent Hamiltonian H is represented as a finite or infinite Hermitian matrix $H_{ij} = H_{ji}^*$ and endowed with an auxiliary dependence on the flow variable s. The application of successive transformations is associated with the forward motion along the s axis such that at the beginning of the flow $H(s = 0)$ matches the original Hamiltonian, while at the end of the flow the matrix $H(s \to +\infty)$ assumes the diagonal form.

Two kinds of flows can be distinguished: In a discrete flow, the flow variable follows a sequence of integer values $s = 0, 1, 2, \ldots$, and in a continuous (or differential) flow, the value of s grows continuously. In the former case, the equation for a single step reads

$$H(s + 1) = U(s)H(s)U^\dagger(s) = e^{\eta(s)}H(s)e^{-\eta(s)}, \qquad (27)$$

where the anti-Hermitian operator $\eta(s) = -\eta^\dagger(s)$ is known as the flow generator. The generator must be constructed in such a way that with each consecutive iteration the Hamiltonian $H(s + 1)$ becomes closer, according to some measure, to the diagonal form than its predecessor $H(s)$. Perhaps the simplest way to diagonalize a finite Hermitian matrix in an iterative manner is to use the Jacobi rotations [54,64]. The algorithm is based on the idea that at each step s one may restrict transformations to a two-dimensional vector space spanned by two basis vectors $|i\rangle$ and $|j\rangle$ and perform a rotation in this subspace so that the off-diagonal elements $H_{ij}(s + 1)$ and $H_{ji}(s + 1)$ vanish and their weight is absorbed into the diagonal elements $H_{ii}(s + 1)$ and $H_{jj}(s + 1)$. Even though subsequent transformations will partially restore previously eliminated matrix elements, all off-diagonal entries will eventually decay to zero.

In analogy to the discrete flow (27), application of a continuous flow also leads to a recursive relation between the Hamiltonians $H(s + ds)$ and $H(s)$, but with an infinitesimal

(close to the identity) unitary transformation

$$H(s + ds) = e^{\eta(s)ds}H(s)e^{-\eta(s)ds}$$
$$= H(s) + [\eta(s), H(s)]ds + O((ds)^2). \quad (28)$$

From Eq. (28) we read off the differential equation representing the evolution of the Hamiltonian

$$\frac{dH(s)}{ds} = [\eta(s), H(s)], \quad (29)$$

where the initial condition $H(0)$ is the original matrix to be diagonalized. The flow generator $\eta(s)$ is typically constructed from the elements of $H(s)$, but the recipe is not unique.

During the flow, the Hamiltonian undergoes only unitary transformations; thus the trace of an integer power p of the matrix $H(s)$ is preserved for any s [54],

$$I_p = \mathrm{Tr}[H^p(s)], \quad (30)$$

with I_p independent of the flow variable s. The case of $p = 2$ (corresponding to the squared Frobenius norm) gives

$$I_2 = \sum_n \sum_m H_{nm}(s)H_{mn}(s)$$
$$= \sum_n H_{nn}^2(s) + \sum_n \sum_{m \neq n} |H_{nm}(s)|^2$$
$$= I_2^{\mathrm{diag}}(s) + I_2^{\mathrm{off}}(s), \quad (31)$$

and because $dI_2/ds = 0$ the diagonal part and the off-diagonal part evolve in opposite ways:

$$\frac{dI_2^{\mathrm{diag}}}{ds} = -\frac{dI_2^{\mathrm{off}}}{ds}. \quad (32)$$

Full diagonalization means $I_2^{\mathrm{off}} = 0$ and is assumed to be achieved at $s \to +\infty$. Thus, the natural requirement for the flow towards diagonalization is to have a non-negative derivative of the diagonal part

$$\frac{dI_2^{\mathrm{diag}}}{ds} \geqslant 0. \quad (33)$$

It turns out that the requirement (33) can be easily fulfilled. Let us write an explicit expression for the derivative in Eq. (33) in terms of the matrix elements [54]

$$\frac{dI_2^{\mathrm{diag}}}{ds} = \sum_n H_{nn}(s)\frac{dH_{nn}(s)}{ds} + \sum_k \frac{dH_{kk}(s)}{ds}H_{kk}(s)$$
$$= \sum_k \sum_{n \neq k}[H_{nn}(s) - H_{kk}(s)]$$
$$\times [\eta_{nk}(s)H_{kn}(s) + \eta_{nk}^*(s)H_{kn}^*(s)]. \quad (34)$$

Note that the contribution from $n = k$ can be omitted because for $n = k$ the expressions in both sets of square brackets are equal to zero: The first expression is obviously zero, while the second one vanishes due to the anti-Hermitian nature of the generator

$$\eta_{nk}(s) = -\eta_{kn}^*(s). \quad (35)$$

One can chose the generator's matrix elements of the form [54]

$$\eta_{nk}(s) = H_{nk}(s)f(H_{nn}(s) - H_{kk}(s)), \quad (36)$$

where $f(x)$ is a real-valued function that must be odd, $-f(x) = f(-x)$, to ensure that the generator will be anti-Hermitian [cf. Eq. (35)]. The purely imaginary diagonal elements of the generator can, without loss of generality, be set to zero, because from Eq. (29) one can see that they do not appear in the evolution of the matrix elements of $H(s)$. Combining Eqs. (36) and (34), we see that the defining condition (33) is satisfied if $xf(x) \geqslant 0$. Let us list three notable choices: $f(x) = x$ gives the canonical Wegner generator [58], $f(x) = 1/x$ was analyzed by White [65], and $f(x) = \mathrm{sgn}(x)$ was used in Ref. [66]. We refer to Ref. [54] for the review of pros and cons of each generator. Note that the requirement (33) does not guarantee the full diagonalization, because at some point the flow may stall, giving $dI_2^{\mathrm{diag}}/ds = dI_2^{\mathrm{off}}/ds = 0$ while I_2^{off} still remains nonzero. For example, all three generators encounter problems in the case of degeneracy, i.e., when $H_{nn}(s) = H_{kk}(s)$ while $H_{nk}(s) \neq 0$.

The generator form in Eq. (36) has a certain disadvantage. If the initial Hamiltonian was represented by a banded matrix (tridiagonal, five diagonal, or similar), this sparse structure would be a nice property to preserve during the course of the flow. However, generators of Eq. (36) do not respect the banded form, and in order to rectify the issue, Mielke [67] proposed the following generator:

$$\eta_{nk}(s) = H_{nk}(s)\mathrm{sgn}(n - k). \quad (37)$$

Note that here the sign function acts not on the matrix elements but on the row and column indices. If the initial Hamiltonian is banded, $H_{nk}(0) = 0$ for $|n - k| > n_0$, this structure survives during the flow. The generator (37) is not of the form of Eq. (36); thus the condition of nondecreasing weight of the diagonal in Eq. (33) is not applicable. However, it was shown [67] that the flow always converges to a final diagonal matrix, even if degeneracies are encountered. Moreover, the diagonal elements are automatically sorted in ascending order, $H_{nn}(+\infty) \geqslant H_{kk}(+\infty)$ for $n > k$. For the special case of real tridiagonal matrices, the generator (37) was previously studied in a different context, namely, the integrable Toda lattice [68]. The name stuck. Shortly, we will define and use a generalized version of the Toda generator to block diagonalize the Kamiltonian (15); therefore, it is natural to call our version the block-diagonalizing Toda generator, or briefly just the Toda generator.

IV. BLOCK DIAGONALIZATION OF THE KAMILTONIAN USING A FLOW APPROACH

The Floquet effective Hamiltonian, defined in Sec. II, can be found by block diagonalizing the Kamiltonian [see Eq. (17)]. Thus, in the present section we will address the problem of block diagonalization of time-dependent Kamiltonians, thus generalizing the flow-based approach of Sec. III which was limited to diagonalization of static Hamiltonians.

There are several differences between diagonalization of a static Hamiltonian and block diagonalization of the Kamiltonian. First, block diagonalization is in fact a much simpler task than the full diagonalization, because a diagonal matrix can be treated as a special case of a block diagonal one but not the other way around. Our goal is to find the FE Hamiltonian $h_{\mathrm{eff}}(t)$, which is not necessarily diagonal with respect to the

basis of the physical space $\mathscr{H}$. This is in contrast to Ref. [69], where the static Kamiltonian is fully diagonalized. Second, the Kamiltonian has a special structure which allows us to write it in terms of the shift operators (15). Thus, we will study only flows that preserve this structure. Third, we consider time-dependent Kamiltonians; therefore, the flow equations (27) and (29) must be generalized to time-dependent matrices. Finally, during the flow we need to keep track of all infinitesimal unitary transformations because they define the overall transformation $\mathcal{D}(t)$ which is used to calculate the micromotion operator (25).

The discrete flow equation (27) can be generalized for time-dependent Kamiltonians as follows:

$$\mathcal{K}(s+1,t) = e^{i\mathcal{S}(s,t)}\mathcal{K}(s,t)e^{-i\mathcal{S}(s,t)} - i\hbar e^{i\mathcal{S}(s,t)}\frac{\partial e^{-i\mathcal{S}(s,t)}}{\partial t}. \tag{38}$$

Here the extended-space operator $i\mathcal{S}$ plays the role of the flow generator and $\mathcal{S}^\dagger = \mathcal{S}$. Correspondingly, the continuous flow Eq. (29) generalizes to [53]

$$\frac{\partial\mathcal{K}(s,t)}{\partial s} = i[\mathcal{S}(s,t),\mathcal{K}(s,t)] - \hbar\frac{\partial\mathcal{S}(s,t)}{\partial t}. \tag{39}$$

We focus exclusively on generators of the form

$$i\mathcal{S}(s,t) = i\sum_{m=-\infty}^{+\infty} P_m \otimes S^{(m)}(s,t), \tag{40}$$

with

$$[S^{(m)}(s,t)]^\dagger = S^{(-m)}(s,t), \tag{41}$$

since this form guarantees that during the flow the Kamiltonian remains of the form set by Eq. (15).

In the case of a discrete flow, the net effect of all unitary transformations can be written as

$$\mathcal{D}^\dagger(t) = e^{i\mathcal{S}(s',t)}e^{i\mathcal{S}(s'-1,t)}\cdots e^{i\mathcal{S}(2,t)}e^{i\mathcal{S}(1,t)}e^{i\mathcal{S}(0,t)}, \tag{42}$$

where s' can be either a finite or an infinite number. For the continuous flow, the joint action of all unitary transformations is written as a flow-ordered integral

$$\mathcal{D}^\dagger(t) = \mathcal{T}_s\exp\left[i\int_0^{+\infty}\mathcal{S}(s,t)ds\right]. \tag{43}$$

A. Generator for discrete flow in the high-frequency regime

Let us analyze a specific example of a discrete flow, considered within the framework of a high-frequency expansion. To be more precise, we assume that $(\hbar\omega)^{-1}$ is a small expansion variable and our goal is to make the Kamiltonian block diagonal up to some order in $(\hbar\omega)^{-1}$. At each step s, the Kamiltonian can be written as

$$\mathcal{K}(s,t) = \hbar\omega N\otimes\mathbf{1}_{\mathscr{H}} + \sum_{m=-\infty}^{+\infty} P_m\otimes H^{(m)}(s,t), \tag{44}$$

where each Fourier component $H^{(m)}(s,t)$ is represented as a power series $H^{(m)}(s,t) = \sum_{i=0}^{+\infty} H_i^{(m)}(s,t)$, with $H_i^{(m)}(s,t)$ being of the order of $(\hbar\omega)^{-i}$. At the start of the flow, $s=0$ and the zeroth-order terms $H_0^{(m)}(0,t)$ are set equal to the original

Fourier components, $H_0^{(m)}(0,t) = h^{(m)}(t)$, while all higher-order terms are zero, $H_{i\geqslant 1}^{(m)}(0,t) = 0$. Moreover, we assume that the time dependence of $h^{(m)}(t)$ is slow in comparison to ω; thus the derivatives behave as $d^j h^{(m)}(t)/dt^j \sim O(1)$ for arbitrary j.

Before we proceed, a comment on notation and terminology is in order. We use the lowercase h to refer to the Fourier harmonics of the driven Hamiltonian as well as of the effective Hamiltonian. They are the input and the output of the flow procedure, respectively. During the flow, we operate with running (that is, s-dependent) Fourier harmonics denoted by uppercase H. We note that Fourier components $H^{(m)}$ with $m\neq 0$ define off-diagonal blocks of the Kamiltonian and thus we will refer to them as the off-diagonal Fourier components. Likewise, $H^{(0)}$ appears only in the diagonal block and thus is the diagonal Fourier component.

Let us assume that it is possible to find a generator that, on each successive application, eliminates the leading term from the expansion of all off-diagonal Fourier components. To be more precise, in the initial ($s=0$) Kamiltonian $\mathcal{K}(0,t)$ the Fourier components $H^{(m\neq 0)}(0,t)$ are represented as series that naturally start with $H_0^{(m\neq 0)}(0,t)$, while at $s=1$ the transformed Kamiltonian $\mathcal{K}(1,t)$ contains Fourier components of $H^{(m\neq 0)}(1,t)$ whose expansion starts with the terms $H_1^{(m\neq 0)}(1,t)$, because $H_0^{(m\neq 0)}(1,t)$ has been set to zero. After two steps of the flow, both $H_0^{(m\neq 0)}(2,t)$ and $H_1^{(m\neq 0)}(2,t)$ are eliminated, and so on. When such a flow reaches a certain value s, one can write

$$\mathcal{K}(s,t) = \hbar\omega N\otimes\mathbf{1}_{\mathscr{H}}$$
$$+ P_0\otimes\sum_{i=0}^{s-1} H_i^{(0)}(s,t) + O\left(\frac{1}{(\hbar\omega)^s}\right), \tag{45}$$

with the obvious interpretation that the Kamiltonian $\mathcal{K}(s,t)$ is block diagonal up to the order $s-1$. Thus the FE Hamiltonian reads $h_{\text{eff}}(t) = \sum_{i=0}^{s-1} H_i^{(0)}(s,t) + O(1/(\hbar\omega)^s)$. Surprisingly, this scenario is realized with a very simple choice of the generator

$$i\mathcal{S}(s,t) = \sum_{m\neq 0}\frac{P_m}{m}\otimes\frac{H_s^{(m)}(s,t)}{\hbar\omega}. \tag{46}$$

For example, at $s=0$ the initial generator reads

$$i\mathcal{S}(0,t) = \sum_{m\neq 0}\frac{P_m}{m}\otimes\frac{h^{(m)}(t)}{\hbar\omega} \tag{47}$$

and after one step of the flow (38) the updated Kamiltonian becomes

$$\mathcal{K}(1,t) = \hbar\omega N\otimes\mathbf{1}_{\mathscr{H}} + P_0\otimes h^{(0)}(t) + O\left(\frac{1}{(\hbar\omega)^1}\right), \tag{48}$$

giving the FE Hamiltonian $h_{\text{eff}}(t) = h^{(0)}(t) + O(1/(\hbar\omega)^1)$.

We have verified that the discrete flow with the generator of the form of Eq. (46) reproduces the high-frequency expansion procedure presented in Ref. [40]. In Appendix A we prove the validity of the generator (46) and also show that the obtained accuracy of Eq. (45) is in fact even better than anticipated.

Let us draw attention to one drawback of the discussed discrete flow driven by the generator (46). Let us say that the initial Hamiltonian $h(\omega t, t)$ has a limited number of contributing Fourier harmonics. In other words, there exists such a positive m_0 that all higher harmonics vanish, i.e., $h^{(m)}(t) = 0$ for $|m| > m_0$. One might expect that during the flow we can restrict the analysis to the limited Fourier spectrum $H^{(m)}(s)$ with $|m| \leqslant m_0$. Unfortunately, that is not true and sooner or later $H^{(m)}(s)$ with $|m| > m_0$ become nonzero. This complicates the automated implementation of the flow using symbolic computation packages. The same drawback is present in the continuous flow discussed in Sec. IV B. Therefore, in Sec. IV C we will proceed to the introduction of the Toda generator, which is not plagued with this problem.

B. Generator proposed by Verdeny, Mielke, and Mintert [37]

Let us now turn to continuous flows to implement the block diagonalization of the Kamiltonian. One can adapt the generator (36) to work with block matrices. By interpreting the partial inner product $\langle n|i\mathcal{S}|k\rangle$ as an element of a block matrix, one can rewrite Eq. (36) in terms of block matrices

$$\langle n|i\mathcal{S}(s,t)|k\rangle = \langle n|\mathcal{K}(s,t)|k\rangle f(\langle n|\mathcal{K}(s,t)|n\rangle - \langle k|\mathcal{K}(s,t)|k\rangle).$$
(49)

Because $\langle n|\mathcal{K}(s,t)|n\rangle = n\hbar\omega \mathbf{1}_{\mathscr{H}} + H^{(0)}(s,t)$, the difference between two diagonal blocks is always proportional to the unit operator. Previously, the function $f(\cdot)$ was defined for real numbers. Here we must slightly generalize the function's action to operators defined in the vector space $\mathscr{H}$ and proportional to the unit operator as $f(x\mathbf{1}_{\mathscr{H}}) = \mathbf{1}_{\mathscr{H}} f(x)$. Thus, with the Wegner case of the function $f(\cdot)$, the generator reads

$$i\mathcal{S}(s,t) = \hbar\omega \sum_{m\neq 0} m P_m \otimes H^{(m)}(s,t).$$
(50)

This generator was proposed in Ref. [37]. Note that because the generator (50) is of the form specified by Eqs. (40) and (41), the Kamiltonian remains of the form set by Eq. (15) during the flow. By substituting Eq. (50) into Eq. (39) we obtain the flow equations for the Fourier components

$$\frac{dH^{(0)}(s,t)}{ds} = \frac{2}{\hbar\omega} \sum_{m=1}^{+\infty} m[H^{(m)}(s,t), H^{(-m)}(s,t)],$$
(51a)

and for $n \neq 0$,

$$\frac{dH^{(n)}(s,t)}{ds} = -n^2 H^{(n)}(s,t) + \frac{i}{\omega} n \dot{H}^{(n)}(s,t)$$
$$+ \frac{1}{\hbar\omega} \sum_{m\neq n} (m-n)[H^{(m)}(s,t), H^{(n-m)}(s,t)].$$
(51b)

Note that here we rescaled the flow variable $s \to s/(\hbar\omega)^2$ for the sake of convenience. The initial conditions for Eq. (51) are $H^{(m)}(0,t) = h^{(m)}(t)$ and the FE Hamiltonian is obtained as the limit $\lim_{s\to+\infty} H^{(0)}(s,t) = h_{\mathrm{eff}}(t)$. Equation (51) can be used as a starting point for approximations. For example, in Appendixes B and C we show how one can obtain the FE Hamiltonian and the micromotion operator in terms of high-frequency expansions when the modulation of the

envelope is slow on the scale set by the driving frequency, i.e., $d^j h^{(m)}(t)/dt^j \sim O(1)$. In principle, such results are a reproduction of the equations obtained in Ref. [40]. A different variant of a high-frequency expansion is obtained in Sec. VI, where we assume a rapid variation of the envelope, i.e., $dh^{(m)}(t)/dt \sim O(\hbar\omega)$. As we will see in Sec. VI, such an assumption places some restrictions on the behavior of the Fourier components as a function of time. The expansion presented in Sec. VI can potentially be useful in situations where the envelope of the perturbation is so fast that only a few oscillations are performed during the perturbation pulse.

C. Block-diagonalizing the Toda generator

As discussed previously, the continuous flow defined by Eq. (51) and the discrete flow presented in Sec. IV A lead to the proliferation of Fourier harmonics $H^{(m)}(s,t)$. In order to overcome this obstacle, we will employ a generator akin to the Toda generator in Eq. (37). In fact, we use the same Eq. (49), but this time with the function $f(x) = \mathrm{sgn}(x)$; thus

$$i\mathcal{S}(s,t) = \sum_{m\neq 0} \frac{\mathrm{sgn}(m)}{\hbar\omega} P_m \otimes H^{(m)}(s,t).$$
(52)

Here we rescale the flow variable $s \to s/(\hbar\omega)^2$ as before. The flow equations produced by the Toda generator (52) are similar to Eq. (51),

$$\frac{dH^{(0)}(s,t)}{ds} = \frac{2}{\hbar\omega} \sum_{m=1}^{+\infty} [H^{(m)}(s,t), H^{(-m)}(s,t)],$$
(53a)

and for $n \neq 0$

$$\frac{dH^{(n)}(s,t)}{ds} = -n\,\mathrm{sgn}(n) H^{(n)}(s,t) + \frac{i}{\omega}\mathrm{sgn}(n)\dot{H}^{(n)}(s,t)$$
$$+ \frac{1}{\hbar\omega} \sum_{m\neq n} \mathrm{sgn}(m-n)$$
$$\times [H^{(m)}(s,t), H^{(n-m)}(s,t)].$$
(53b)

In Appendix E we show that if the initial condition $H^{(n)}(0,t) = 0$ for $|n| > n_0$, then $H^{(n)}(s,t) = 0$ for all $s \in [0, +\infty)$. This feature facilitates an automated generation of a high-frequency expansion from the flow Eqs. (53).

V. AUTOMATED EXPANSION FOR A FINITE CLOSED ALGEBRA

Appendixes B and C describe the procedure that allows us to derive the FE Hamiltonian and the micromotion operator starting from Eqs. (53) in the high-frequency regime, including the possibility of a slow modulation of the driving amplitude. However, manual implementation of this procedure for expansions of higher order is too tedious. Mikami *et al.* [38] were able to write out such an expansion up to the fourth order for the simpler case of unmodulated periodic driving. The authors of Refs. [48,49] were able to proceed to even higher orders within the framework of the Magnus-Taylor expansion and specializing to a two-level system. Here we demonstrate that an automated expansion to an arbitrary order (limited only by the available computational

resources) can be achieved with the help of a symbolic computational package. However, for this scheme to succeed, we need to place several restrictions on the initial Hamiltonian $h(\omega t + \theta, t)$. Namely, we assume that the Hamiltonian has a limited number of Fourier harmonics, that is, $h^{(n)}(t) = 0$ for $|n| > n_0$, and the Hamiltonian is written in terms of a finite L-dimensional Lie algebra spanned by the Hermitian generators G_l with $l = 1, 2, \ldots, L$. Thus

$$h^{(n)}(t) = \sum_{l=1}^{L} c_l^{(n)}(t) G_l \qquad (54)$$

and the functions $c_l^{(n)}(t)$ are complex-valued functions of time. In the absence of the additional modulation of the driving signals they reduce to mere complex numbers. The algebra is closed with respect to the commutator

$$[G_l, G_m] = \sum_{n=1}^{L} \gamma_{lmn} G_n, \qquad (55)$$

where γ_{lmn} are the structure constants defined by the algebra. Note that in general the algebra can be closed in an approximate sense: Certain terms produced by the commutator (54) are ignored as not belonging to the model considered. The simplest nontrivial example is provided by a two-level system or a spin-$\frac{1}{2}$ particle in a magnetic field. Here one operates within the algebra with $L = 3$ generators $\sigma_{\{x,y,z\}}$ represented by the Pauli matrices and the structure constant $\gamma_{lmn} = 2i\epsilon_{lmn}$ proportional to the Levi-Cività antisymmetric tensor. Thus the commutators in Eq. (53) can be expressed in terms of products of coefficients $c_l^{(n)}(t)$. By expanding the coefficients in power series of the inverse frequency $c_l^{(n)}(t) = c_{l,0}^{(n)}(t) + c_{l,1}^{(n)}(t) + \cdots$, a symbolic computation package can collect terms of the same order on both sides of the flow equations and solve the ensuing differential equations order by order for $c_{l,j}^{(n)}(s, t)$. Note that the differential equations produced during this procedure are nothing more than linear inhomogeneous first-order differential equations [see, for example, Eq. (B9)], thus easily solvable with a symbolic computation package. The micromotion operator is obtained in a similar way; in this case one computes the integrals generated by the Magnus

expansion. Each consecutive term in the expansion is obtained from the exact recursive relations given in Ref. [62].

To give a concrete example of an automated construction of a high-frequency expansion, we consider the case of the su(2) algebra, specifically, the Rabi model subject to a linearly polarized drive (alternative expansions for the same model were analyzed in Refs. [48,49])

$$h_{\text{lab}}(\omega t, t) = \frac{\hbar\Omega}{2}\sigma_z + 2g(t)\cos(\omega t + \phi)\sigma_x. \qquad (56)$$

Here we assume that Ω is comparable to ω, more precisely, we assume a small detuning $\hbar\Omega - \hbar\omega = \Delta \sim O(1)$. Therefore, the original Hamiltonian (56) is not suitable to proceed with the inverse frequency expansion, and we first transition into a moving frame with the help of the unitary transformation $\tilde{U}(t) = \exp[-i\omega t \sigma_z/2]$. The transformed Hamiltonian reads

$$\begin{aligned} h(\omega t, t) &= \tilde{U}^\dagger(t) h_{\text{lab}}(\omega t, t)\tilde{U}(t) - i\hbar\tilde{U}^\dagger(t)\frac{d\tilde{U}(t)}{dt} \\ &= \frac{\Delta}{2}\sigma_z + g(t)[\cos(\phi) + \cos(2\omega t + \phi)]\sigma_x \\ &\quad + g(t)[\sin(\phi) - \sin(2\omega t + \phi)]\sigma_y \end{aligned} \qquad (57)$$

and the contributing nonzero Fourier components are

$$h^{(0)} = \frac{\Delta}{2}\sigma_z + g(t)\cos(\phi)\sigma_x + g(t)\sin(\phi)\sigma_y, \qquad (58a)$$

$$h^{(2)} = \frac{g(t)}{2}e^{i\phi}\sigma_x + \frac{g(t)}{2}ie^{i\phi}\sigma_y = [h^{(-2)}]^\dagger. \qquad (58b)$$

Explicit expansion formulas for the FE Hamiltonian are quite bulky; therefore, in Appendix F we present a truncated expansion up to the fourth order with $\phi = 0$. Here we limit ourselves to the second-order expansions. The effective Hamiltonian reads

$$\begin{aligned} h_{\text{eff}} &= \sigma_x\left[g(t)\cos\phi - \frac{g^3(t)\cos\phi}{4(\hbar\omega)^2}\right] \\ &\quad + \sigma_y\left[g(t)\sin\phi - \frac{g^3(t)\sin\phi}{4(\hbar\omega)^2}\right] \\ &\quad + \sigma_z\left[\frac{\Delta}{2} + \frac{g^2(t)}{2\hbar\omega} - \frac{\Delta g^2(t)}{4(\hbar\omega)^2}\right] \end{aligned} \qquad (59a)$$

and the micromotion is given by $U_{\text{micro}}(t) = e^{-iS(t)}$, with

$$\begin{aligned} S(t) &= \sigma_x\left[\frac{g(t)\sin(2\omega t + \phi)}{2\hbar\omega} - \frac{\Delta g(t)\sin(2\omega t + \phi)}{4(\hbar\omega)^2} + \frac{\hbar g'(t)\cos(2\omega t + \phi)}{4(\hbar\omega)^2}\right] \\ &\quad + \sigma_y\left[\frac{g(t)\cos(2\omega t + \phi)}{2\hbar\omega} - \frac{\Delta g(t)\cos(2\omega t + \phi)}{4(\hbar\omega)^2} - \frac{\hbar g'(t)\sin(2\omega t + \phi)}{4(\hbar\omega)^2}\right] + \sigma_z\frac{g^2(t)\sin(2\omega t + 2\phi)}{2(\hbar\omega)^2}. \end{aligned} \qquad (59b)$$

In contrast to Refs. [48,49], in our expansions the first- and second-order FE Hamiltonians do not depend on the time derivative $g'(t)$. The reason for this is that the expansion is performed for different Hamiltonians: the FE Hamiltonian in our case and the FS Hamiltonian in the example of Refs. [48,49].

Figure 1 shows the results of a numerical simulation based on the obtained high-frequency expansion given in Eq. (59).

We focus on a two-level system described by the Hamiltonian (57) with the parameters $g(t) = \text{const}$, $\Delta/\hbar\omega = 0.3$, $g/\hbar\omega = 0.2$, and $\phi = 0$ and initially prepared in the ground state. Using a number of different approximations, we compute the probability $P_{1\to2}$ of transition to the excited state as a function of the scaled time ωt. In Fig. 1(a) we cover the time interval $\omega t \in [0, 60]$ that roughly corresponds to five Rabi cycles, and
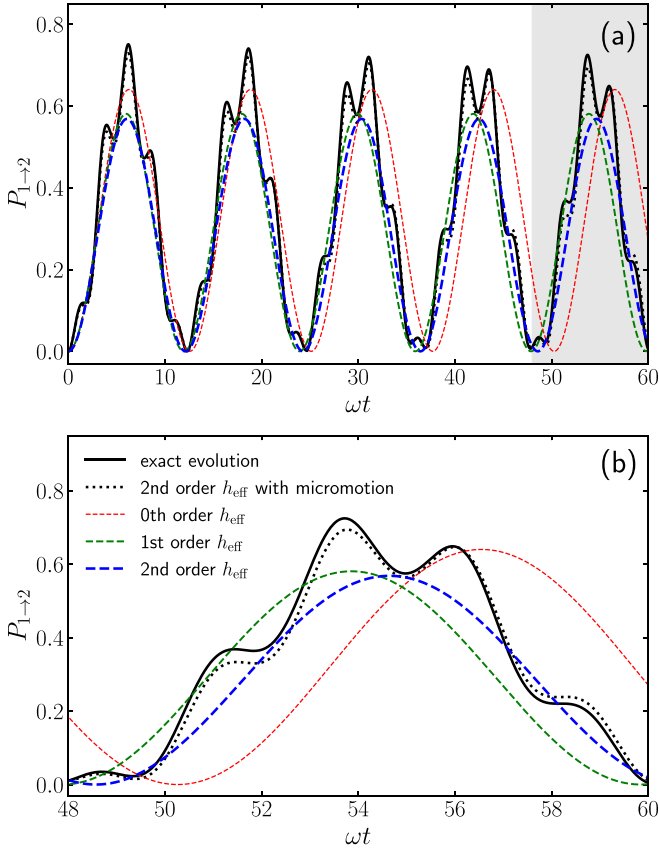
FIG. 1. Probability of transition to the excited state in a driven two-level system, calculated using various approximations. The numerically exact evolution (solid line) is reliably reproduced only when the micromotion is included (dotted line). Approximations that do not take micromotion into account (dashed lines) consistently fail to reproduce full details of the evolution

Fig. 1(b) shows a magnification of the last cycle marked by the shaded area in Fig. 1(a). The black solid line shows the exact evolution, obtained from numerical time propagation of the time-dependent Schrödinger equation using a fourth-order Runge-Kutta scheme. The black dotted line corresponds to the approximate evolution calculated using the complete information available from Eq. (59), i.e., including both the effective Hamiltonian (59a) and the micromotion (59b). To elucidate the role of particular terms, we include three dashed lines corresponding to approximations that neglect the micromotion and truncate the effective Hamiltonian. The different levels of approximation are encoded using the color and thickness of the dashed lines. The thinnest red line depicts the evolution generated by including only the zeroth-order terms in the effective Hamiltonian and the green line of intermediate thickness corresponds to the case when the zeroth- and first-order terms are included. Finally, the thickest blue dashed line corresponds to the second-order approximation for the effective Hamiltonian (59a), however still not taking the micromotion into account. We see that improved accuracy of the effective Hamiltonian translates to a more reliable calculation of the period of the Rabi cycle; however, inclusion of the micromotion is indeed essential for the reliable description of the complete quantum evolution.

VI. CASE OF FAST AMPLITUDE MODULATION

Let us now return to the flow Eqs. (51) and perform the inverse-frequency expansion analogous to that presented in Appendixes B and C, however focusing on the case of fast amplitude modulation. We now assume that the rate of change of the Fourier components of the driven Hamiltonian is comparable to the driving frequency, formally expressed as $d^j h^{(m)}(t)/dt^j \sim O(\omega^j)$. Although it may seem that in such a regime the frequency can no longer be considered high, we stress that the amplitudes of the Fourier components are still assumed to be low, $h^{(m)}(t) \sim O(1)$.

Repeating the steps in Appendix B, we expand each Fourier component into an inverse-frequency power series $H^{(n)}(s, t) = H_0^{(n)}(s, t) + H_1^{(n)}(s, t) + \cdots$, insert the expansions into the flow Eqs. (51), and collect terms of the same order on both sides. In the zeroth order we get a trivial equation for the zeroth Fourier component,

$$\frac{dH_0^{(0)}}{ds} = 0, \tag{60a}$$

and a modified equation for the $n \neq 0$ Fourier components,

$$\frac{dH_0^{(n)}(s, t)}{ds} = -n^2 H_0^{(n)}(s, t) + \frac{i}{\omega} n \dot{H}_0^{(n)}(s, t). \tag{60b}$$

From the trivial Eq. (60a) we find the zeroth-order FE Hamiltonian $h_{\text{eff}(0)}(t) = h^{(0)}(t)$, while the first-order FE Hamiltonian $h_{\text{eff}(1)}(t)$ can be obtained by solving Eq. (60b). In principle, Eq. (60b) is a partial differential equation, because derivatives with respect to s and t act on the same quantity. Such an equation can be solved using an additional Fourier expansion with respect to t. We are interested in the time interval $t \in [t_{\text{in}}, t_{\text{fn}}]$ and assume that the driven Hamiltonian is the same on the boundaries of the interval, $h^{(n)}(t_{\text{in}}) = h^{(n)}(t_{\text{fn}})$. Thus the Fourier expansion with respect to t reads

$$H_0^{(n)}(s, t) = \sum_{j=-\infty}^{+\infty} H_0^{(n,j)}(s) \exp[ij\Omega t], \tag{61}$$

where $\Omega = 2\pi/(t_{\text{fn}} - t_{\text{in}})$ is the characteristic frequency of the envelope. In view of $[H_0^{(n)}]^\dagger = H_0^{(-n)}$ we have

$$\left[H_0^{(n,j)}(s)\right]^\dagger = H_0^{(-n,-j)}(s). \tag{62}$$

Each Fourier component of the original Hamiltonian can be expanded into a Fourier series $h^{(n)}(t) = \sum_j h^{(n,j)} \exp[ij\Omega t]$; thus at the beginning of the flow we have $H_0^{(n,j)}(0) = h^{(n,j)}$. Substituting the ansatz (61) into the flow Eq. (60b), one can see that different Fourier components (for different j) do not couple

$$\frac{dH_0^{(n,j)}(s)}{ds} = -n^2 H_0^{(n,j)}(s) - \frac{\Omega}{\omega} jn H_0^{(n,j)}(s) \tag{63}$$

and are described by the exponential solutions

$$H_0^{(n,j)}(s) = h^{(n,j)} \exp\left[-\left(n^2 + \frac{\Omega}{\omega} jn\right)s\right]. \tag{64}$$

The high-frequency expansion converges only if $H_0^{(n,j)}(s \to +\infty) = 0$. Therefore, one should place a restriction on the index j. We assume that the expansion of the envelope (61) does not have high harmonics

$$H_0^{(n)}(s,t) = \sum_{j=-J}^{J} H_0^{(n,j)}(s) \exp[ij\Omega t], \qquad (65)$$

and the positive integer J satisfies

$$J < \frac{\omega}{\Omega}. \qquad (66)$$

This means that if, over the interval $[t_{\text{in}}, t_{\text{fn}}]$, the high-frequency modulation oscillates $J + \varepsilon$ times [here $\varepsilon \in (0,1)$], then the expansion of the envelope cannot have harmonic number higher than J. For example, if the high-frequency modulation oscillates 3.5 times, then the shape of the envelope expanding into the Fourier series cannot possess the fourth harmonic.

Next, using the expansion (65), one can write the first-order flow equation for the zeroth Fourier component

$$\frac{dH_1^{(0)}(s,t)}{ds} = \frac{2}{\hbar\omega} \sum_{m=1}^{+\infty} \sum_{j=-J}^{J} \sum_{j'=-J}^{J} m[h^{(m,j)}, h^{(-m,j')}]e^{i(j+j')\Omega t} e^{-[2m^2 + m(\Omega/\omega)(j-j')]s}. \qquad (67)$$

Integrating this equation and taking into account the initial condition $H_1^{(0)}(0,t) = 0$, we obtain the solution. Calculation of the limit $s \to +\infty$ yields the first-order FE Hamiltonian

$$h_{\text{eff}(1)}(t) = \frac{1}{\hbar\omega} \sum_{m=1}^{+\infty} \sum_{j=-J}^{J} \sum_{j'=-J}^{J} \frac{[h^{(m,j)}, h^{(-m,j')}]}{m + \frac{\Omega}{2\omega}(j - j')} e^{i(j+j')\Omega t}. \qquad (68)$$

We obtained the FE Hamiltonian up to the first order. Let us now calculate the corresponding first-order expansion of the micromotion operator. The procedure is similar to that presented in Appendix C, because we use the same generator form (C2) as in Appendix C. The equations up to Eq. (C4) are identical; thus $\mathcal{S}_0 = 0$. Yet the first-order correction, taking into account the solution (64), reads

$$\mathcal{S}_1(t) = \frac{1}{i\hbar\omega} \sum_{m\neq 0} P_m \otimes \sum_{j=-J}^{J} \frac{h^{(m,j)}e^{ij\Omega t}}{m + \frac{\Omega}{\omega}j}. \qquad (69)$$

The micromotion operator in the physical space $\mathscr{H}$ reads

$$U_{\text{micro}}^{\dagger}(\omega t + \theta, t) = \exp\left[\frac{1}{\hbar\omega} \sum_{m\neq 0} \left\{\frac{e^{im(\omega t + \theta)}}{m} \sum_{j=-J}^{J} \frac{h^{(m,j)}e^{ij\Omega t}}{1 + \frac{\Omega}{\omega}\frac{j}{m}}\right\} + O\left(\frac{1}{(\hbar\omega)^2}\right)\right]. \qquad (70)$$

Because of Eq. (66) we have $|\Omega j/\omega m| < 1$, and using the geometric progression series $1/(1 + x) = 1 - x + x^2 - \cdots$ we can rewrite Eq. (70) in terms of the full Fourier harmonics $h^{(m)}(t)$ and its derivatives as

$$U_{\text{micro}}^{\dagger}(\omega t + \theta, t) = \exp\left[\frac{1}{\hbar\omega} \sum_{m\neq 0} \left\{\frac{e^{im(\omega t + \theta)}}{m} \sum_{l=0}^{+\infty} \left(\frac{i}{\omega m}\frac{d}{dt}\right)^l h^{(m)}(t)\right\} + O\left(\frac{1}{(\hbar\omega)^2}\right)\right]. \qquad (71)$$

From this expression one can see that if at the time moments $t = \{t_{\text{in}}, t_{\text{fn}}\}$ the amplitude of the envelope equals zero, $h^{(m\neq 0)}(t) = 0$, then the micromotion operator still does not equal unity, because of the derivatives of the Fourier components $d^l h^{(m\neq 0)}(t)/dt^l \neq 0$ of various orders. This result differs from the expansion presented in Appendix C, where the first-order micromotion operator (C4) does not contain derivatives, the second-order micromotion operator (C7) has only first derivative, and so on.

Similarly to Eq. (71), one can rewrite the first-order FE Hamiltonian (68) in the terms of the full Fourier component $h^{(m)}(t)$ instead of the double-indexed Fourier components $h^{(m,j)}$. To do that we again use the geometric series for the fraction

$$\frac{1}{m + \frac{\Omega}{2\omega}(j - j')} = \frac{1}{m}\left[1 + \frac{i^2\Omega(j - j')}{2\omega m} + \left(\frac{i^2\Omega(j - j')}{2\omega m}\right)^2 + \cdots\right]. \qquad (72)$$

Then, in the terms of $h^{(m)}(t)$ and its derivatives, the first-order FE Hamiltonian reads

$$h_{\text{eff}(1)}(t) = \frac{1}{\hbar\omega} \sum_{m\neq 0} \frac{1}{2m} \sum_{l=0}^{+\infty} \left(\frac{i}{2\omega m}\right)^l \sum_{r=0}^{l} \frac{l!(-1)^r}{r!(l-r)!}\left[\frac{d^{(l-r)}h^{(m)}(t)}{dt^{(l-r)}}, \frac{d^r h^{(-m)}(t)}{dt^r}\right]. \qquad (73)$$

This expression is consistent with Eq. (B13). To be more precise, we can reproduce the term proportional to $[\dot{h}^{(m)}, h^{(-m)}]$. Let us take only $l = 0$ and $l = 1$ in Eq. (73). Then it reads

$$
h_{\text{eff}(1)}(t) \approx \sum_{m=1}^{+\infty} \frac{[h^{(m)}(t), h^{(-m)}(t)]}{m\hbar\omega} + \frac{1}{(2\hbar\omega)^2} \sum_{m \neq 0} \frac{i\hbar}{m^2} \{[\dot{h}^{(m)}(t), h^{(-m)}(t)] - [h^{(m)}(t), \dot{h}^{(-m)}(t)]\}
$$

$$
= \sum_{m=1}^{+\infty} \frac{[h^{(m)}(t), h^{(-m)}(t)]}{m\hbar\omega} + \sum_{m \neq 0} \frac{i\hbar[\dot{h}^{(m)}(t), h^{(-m)}(t)]}{2(\hbar\omega)^2 m^2}. \tag{74}
$$

If we assume that the additional time dependence is slow, such that $\dot{h}^{(m)} \sim O(1)$, the second term of Eq. (74) becomes second order and it is exactly equal to the term responsible for the non-Abelian geometric phase [40] in quantum systems where $[\dot{h}^{(m)}, h^{(-m)}] \neq 0$. Note that Eq. (73) contains not only first-order but also higher-order derivatives; thus it can be used to engineer unusual effects.

VII. EXAMPLES

In this section we describe several examples of high-frequency expansion for specific operator algebras.

A. Spin-$\frac{1}{2}$ particle in an oscillating and slowly rotating magnetic field

We begin by revisiting the model discussed in Refs. [40,70] as the simplest example of a driven system where nontrivial behavior emerges from the modulation of the drive. The scaled driven Hamiltonian reads

$$
h(\omega t, t) = [B_x(t)\sigma_x + B_y(t)\sigma_y]\cos\omega t \tag{75}
$$

and describes a spin-$\frac{1}{2}$ particle in a rapidly oscillating magnetic field (the frequency ω sets the dominant scale) whose amplitude is also slowly changing as a function of time. Here the Hamiltonian and the magnetic field are measured in the units of the frequency. The envelope is parametrized by the two projections $B_x(t)$ and $B_y(t)$. Its magnitude $[B_x^2(t) + B_y^2(t)]^{1/2}$ is of little interest to our purposes, but the direction must be changing as a function of time. Thus, $B_x(t)$ and $B_y(t)$ must be distinct functions, i.e., we will take that they are not equal or proportional. Automated generation of the effective Hamiltonian up to the fourth order in the inverse frequency gives

$$
h_{\text{eff}(0)} = h_{\text{eff}(1)} = h_{\text{eff}(3)} = 0, \tag{76a}
$$

$$
h_{\text{eff}(2)}(t) = \sigma_z 2[B_x(t)B_y'(t) - B_y(t)B_x'(t)]\omega^{-2}, \tag{76b}
$$

$$
h_{\text{eff}(4)}(t) = \sigma_z \left\{ \frac{1}{2}B_x'''B_y - \frac{1}{2}B_xB_y''' \right.
$$
$$
+ B_x'\left[2B_x^2B_y + \frac{3B_y''}{2} + 2B_y^3\right]
$$
$$
\left. - B_y'\left[2B_xB_y^2 + \frac{3B_x''}{2} + 2B_x^3\right] \right\}\omega^{-4}. \tag{76c}
$$

In Eq. (76c) we skipped the time argument for brevity. As the zeroth and the first terms vanish, the leading term is given

by Eq. (76b). This term can be expressed as

$$
H = 2\omega^{-2}(\boldsymbol{B} \times \dot{\boldsymbol{B}}) \cdot \boldsymbol{\sigma}, \tag{77}
$$

with $\boldsymbol{B} = \boldsymbol{e}_x B_x(t) + \boldsymbol{e}_y B_y(t)$, and reproduces the result of Ref. [40]. The availability of automated expansion allows us obtain also the subleading term behaving as ω^{-4} and featuring higher-order derivatives and their combinations. We note that all terms in Eq. (76) are proportional to derivatives and vanish identically in the absence of temporal modulation.

B. Minimal many-body system

In this example, we discuss a minimal many-body system of two interacting bosonic particles populating a dimer consisting of two lattice sites. We introduce the creation (annihilation) operators $c_j^\dagger$ (c_j), with the subscript $j \in \{1, 2\}$ corresponding to the site number, and write the driven Hamiltonian as

$$
h(\omega t, t) = J(\omega t, t)\tau_1 + \frac{\Delta(\omega t, t)}{2}\tau_3 + \frac{U}{2}\tau_4, \tag{78}
$$

with the operators

$$
\tau_1 = \hat{c}_1^\dagger \hat{c}_2 + \hat{c}_2^\dagger \hat{c}_1, \tag{79a}
$$

$$
\tau_3 = \hat{c}_2^\dagger \hat{c}_2 - \hat{c}_1^\dagger \hat{c}_1, \tag{79b}
$$

$$
\tau_4 = \hat{c}_1^\dagger \hat{c}_1^\dagger \hat{c}_1 \hat{c}_1 + \hat{c}_2^\dagger \hat{c}_2^\dagger \hat{c}_2 \hat{c}_2. \tag{79c}
$$

The three parts of the Hamiltonian (78) describe the hopping transitions with a time-dependent transition strength J, the difference of on-site energies Δ, and bosonic on-site interaction of strength U, respectively. We list also the remaining operators that will be needed to describe the effective dynamics:

$$
\tau_2 = i(\hat{c}_1^\dagger \hat{c}_2 - \hat{c}_2^\dagger \hat{c}_1), \tag{79d}
$$

$$
\tau_5 = i(n_2 \hat{c}_1^\dagger \hat{c}_2 + n_1 \hat{c}_2^\dagger \hat{c}_1) + \text{H.c.}, \tag{79e}
$$

$$
\tau_6 = n_2 \hat{c}_1^\dagger \hat{c}_2 - n_1 \hat{c}_2^\dagger \hat{c}_1 + \text{H.c.}, \tag{79f}
$$

$$
\tau_7 = n_1 n_2, \tag{79g}
$$

$$
\tau_8 = \hat{c}_1^\dagger \hat{c}_1^\dagger \hat{c}_2 \hat{c}_2 + \hat{c}_2^\dagger \hat{c}_2^\dagger \hat{c}_1 \hat{c}_1, \tag{79h}
$$

$$
\tau_9 = i(\hat{c}_2^\dagger \hat{c}_2^\dagger \hat{c}_1 \hat{c}_1 - \hat{c}_1^\dagger \hat{c}_1^\dagger \hat{c}_2 \hat{c}_2). \tag{79i}
$$

Here $n_j = \hat{c}_j^\dagger \hat{c}_j$.

The collection of operators τ_n is closely related, albeit not in one-to-one correspondence, to the su(3) algebra spanned by the Gell-Mann matrices. To see this, we define the basis of three two-particle states

$$
|1\rangle = \frac{1}{\sqrt{2}}\hat{c}_1^\dagger \hat{c}_1^\dagger |\emptyset\rangle, \tag{80a}
$$

$$|2\rangle = \hat{c}_1^\dagger \hat{c}_2^\dagger |\emptyset\rangle, \tag{80b}$$

$$|3\rangle = \frac{1}{\sqrt{2}} \hat{c}_2^\dagger \hat{c}_2^\dagger |\emptyset\rangle. \tag{80c}$$

where $|\emptyset\rangle$ denotes the vacuum state. In this basis, the operators τ_n are encoded as matrices that are simple combinations of the Gell-Mann matrices λ_m and the 3×3 unit matrix. For example, τ_1 and τ_6 are represented as

$$\tau_{1|6} = \begin{pmatrix} 0 & \pm\sqrt{2} & 0 \\ \pm\sqrt{2} & 0 & \sqrt{2} \\ 0 & \sqrt{2} & 0 \end{pmatrix} = \frac{\lambda_6 \pm \lambda_1}{\sqrt{2}}, \tag{81}$$

with the upper (lower) sign for τ_1 (τ_6). Note that the physical content of the model requires that the unit matrix is also included: Interactions are described in terms of matrices τ_4 (on-site interaction) and τ_7 (neighbor interactions) that have nonzero traces. The introduced matrix representations allow for an easy calculation of the commutator algebra and its implementation in a symbolic computation system.

To give an example, we assume that the shaking protocol is such that

$$J(\omega t, t) = j_0 + 2 j_1(t) \cos \omega t, \tag{82a}$$

$$\Delta(\omega t, t) = \delta_0 = \text{const}, \tag{82b}$$

that is, the on-site energy splitting is a constant set to δ_0, whereas the hopping matrix element is harmonically modulated in time around some average value j_0. The factor 2 is included in Eq. (82a) to account for the fact that $2 \cos \omega t = e^{i\omega t} + e^{-i\omega t}$ so that $j_1(t)$ has the meaning of the modulated first Fourier component.

We obtain the effective Hamiltonian in the form of a high-frequency expansion

$$h_{\text{eff}} = \sum_{l=1}^{9} \tau_l (c_{l,0} + c_{l,2} + c_{l,4} + \cdots), \tag{83}$$

with $c_{l,i} \sim O(\omega^{-i})$. Note that first- and third-order terms vanish. In the zeroth order, quite obviously, only time averages are present

$$c_{1,0} = j_0, \quad c_{3,0} = \delta_0, \quad c_{4,0} = \frac{U}{2}, \tag{84}$$

and the remaining coefficients $c_{l,0} = 0$ with $l \in \{2, 5, 6, 7, 8, 9\}$.

In the second order, we find four nonzero contributions

$$c_{3,2} = -\frac{4\delta_0 j_1^2(t)}{(\hbar\omega)^2}, \tag{85a}$$

$$c_{4,2} = -\frac{2U j_1^2(t)}{(\hbar\omega)^2}, \tag{85b}$$

$$c_{7,2} = \frac{8U j_1^2(t)}{(\hbar\omega)^2}, \tag{85c}$$

$$c_{8,2} = -\frac{2U j_1^2(t)}{(\hbar\omega)^2}. \tag{85d}$$

Interestingly, Eq. (85b) shows that shaking has led to a renormalization of the on-site interaction strength from U to

$U - \Delta U$, with $\Delta U = 4U j_1^2(t)/(\hbar\omega)^2$. This is easy to interpret in terms of a process where a particle is able to jump twice during the period of the drive: Two particles that share a site in fact spend some fraction of the period sitting on separate sites and thus not interacting. Likewise, as a consequence of the same process, Eq. (85c) shows that shaking has led to the engineering of hitherto absent nearest-neighbor interactions: Two particles sitting on neighboring sites experience an interaction energy of magnitude $V = 2\Delta U$. The factor 2 comes from the fact that in the considered dimer two sites share a single link. The appearance of modified interactions with a similar sum rule can be generalized to large lattices as discussed in Refs. [34,71]. A similar expression in Eq. (85d) shows that the described process is also responsible for the appearance of pair tunnelings expressed by the operator τ_8. Finally, from Eq. (85a) we also learn that the difference of on-site energies is also weakened. This effect is not related to interactions; thus the modification is proportional to δ_0 rather than U (as seen in previous cases). However, the proportionality to $j_1^2(t)$ is still present, revealing that a sequence of two hopping transitions during the period of the drive is involved. The remaining second-order contributions are zero; thus $c_{l,2} = 0$ for $l \in \{1, 2, 5, 6, 9\}$.

In the fourth order of the high-frequency expansion we find further modifications to the terms already affected in the second order: The coefficients $c_{3,4}$, $c_{4,4}$, $c_{7,4}$, and $c_{8,4}$ are all nonzero. However, these effects are not the leading ones; they are dwarfed by the presence of already discussed processes and therefore are not so interesting. Let us just mention that they feature combinations of the time derivatives such as $j_1''(t)$ and $[j_1'(t)]^2$ as a key prediction of the presented high-frequency expansion for systems with the time-modulated drive.

In addition, we find two more fourth-order contributions to the effective Hamiltonian

$$c_{1,4} = -\frac{12 j_0 j_1^2(t)(\delta_0^2 + U^2)}{(\hbar\omega)^4}, \tag{86a}$$

$$c_{6,4} = -\frac{10 j_0 j_1^2(t)\delta_0 U}{(\hbar\omega)^4}. \tag{86b}$$

The former signals the reduction of the hopping matrix element, while the latter is an indication of density-assisted tunneling events captured by τ_6. These processes are however best explored on large lattices, that is beyond, the overly restrictive dimer model.

The consideration of an alternative [to Eq. (82)] shaking protocol that modifies on-site energies, i.e., Δ, rather than the hopping strengths

$$J(\omega t, t) = j_0 = \text{const}, \tag{87a}$$

$$\Delta(\omega t, t) = \delta_0 + 2\delta_1(t) \cos \omega t \tag{87b}$$

is conceptually similar. In the fourth order it delivers a number of contributions that are leading, i.e., not dwarfed by the second-order contributions. (The first and the third order still vanish). For example, the renormalized on-site interaction energy is

$$U_{\text{eff}} = U - \frac{12 j_0^2 U \delta_1^2(t)}{(\hbar\omega)^4} + O((\hbar\omega)^{-6}). \tag{88}$$

In the second order, the only effect is the well-known [3] modification of the tunneling strength

$$j_{\text{eff}} = j_0 \left[1 - \left(\frac{2\delta_1(t)}{\hbar\omega} \right)^2 + O((\hbar\omega)^{-4}) \right] \qquad (89)$$

by the Bessel function of the zeroth order, identifiable by the leading terms of its power series.

VIII. CONCLUSION

To summarize, the flow-equation approach is a versatile tool useful in the study of driven quantum systems. This method accomplishes a gradual transformation of the given Hamiltonian from its original form to the desired (diagonal or block-diagonal) final form. The flow is implemented by introducing an auxiliary flow variable and specifying an anti-Hermitian generator that expresses the law of motion along the flow variable. In our work we demonstrated the applicability of such a scheme to the block diagonalization of Kamiltonian (quasienergy) matrices that describe driven quantum systems in the extended-space formalism. Importantly, we consider situations where the time dependence is twofold: The system is driven be a force of a certain frequency and its amplitude is additionally modulated as a function of time. Thus, the drive is described as a superposition of a number of Fourier harmonics whose amplitudes are time dependent. The outcome of the flow procedure is the Floquet effective Hamiltonian and the complementary micromotion operator that allow us to faithfully describe the system's time evolution. Alongside a previously proposed Verdeny-Mielke-Minter generator [37], we introduced a modified (Toda) generator (52) that leads to similar flow Eqs. (53) but also guarantees that the spectrum of the contributing Fourier harmonics does not broaden beyond what was present in the driven Hamiltonian. We note that the above procedure in principle applies to both slow and rapid modulation of the amplitude of the drive. However, concrete expressions for the effective Hamiltonian and the micromotion operator were obtained from the high-frequency expansion that assumes that driving frequency sets the dominant scale. The feature of nonproliferation of the Fourier harmonics during the flow is particularly useful when enlisting the help of computer algebra systems to obtain automated high-frequency expansions for the effective Hamiltonian and the micromotion operator. Such expansions are cumbersome to perform manually beyond a few leading terms. We showed that in the case when the Hamiltonian is spanned by a finite Lie algebra, the derivation of the high-frequency expansion can be straightforwardly implemented based on the automated solution of a set of linear inhomogeneous differential equations. The applicability of such a strategy is supported by studying a selection of examples: a spin-$\frac{1}{2}$ particle in an oscillating and slowly rotating magnetic field, a minimal many-body system consisting of two interacting bosons on a driven dimer, and a two-level system subject to a linearly polarized drive.

ACKNOWLEDGMENTS

APPENDIX A: VALIDITY OF THE GENERATOR FOR DISCRETE FLOW

Let us consider a discrete flow indexed by an integer-valued variable running from zero to infinity and assume that having reached a particular value of s, the Kamiltonian has the form

$$\mathcal{K}(s) = \hbar\omega N \otimes \mathbf{1}_{\mathscr{H}} + P_0 \otimes \sum_{i=0}^{+\infty} H_i^{(0)}(s)$$

$$+ \sum_{m\neq 0} \left(P_m \otimes \sum_{i=s}^{+\infty} H_i^{(m)}(s) \right). \qquad (A1)$$

Here, in the off-diagonal part of the Kamiltonian the power series of Fourier components $H^{(m)}$ with $m \neq 0$ start from the order s, that is, the terms that behave as $(\hbar\omega)^{-i}$ with $i \in [0, s-1]$ have already been eliminated. For the sake of simplicity, in this section we will not write the explicit dependence on time, but will keep it in mind. Now we want to demonstrate that the application of the following step of the flow governed by Eq. (38) with the generator (46) will move the Kamiltonian forward along the flow: The flow variable will reach the value $s+1$ and the power series of the Fourier components will start from the order $s+1$. Thus, the general form of Eq. (A1) will be maintained subject to relabeling $s \to s+1$. Note that the generator (46) is of the order $(\hbar\omega)^{-(s+1)}$, but is combined with the first term on the right-hand side of Eq. (A1) which is proportional to $\hbar\omega$. This allows us to eliminate the sth $-$ order terms. Of course, during the considered $s \to s+1$ step, the flow will modify not only terms of orders s and $s+1$, but higher-order terms as well. However, in order to prove our statement it is sufficient to focus on terms that behave as $(\hbar\omega)^{-s}$ and $(\hbar\omega)^{-(s+1)}$. Let us expand the first term in Eq. (38),

$$e^{i\mathcal{S}(s)}\mathcal{K}(s)e^{-i\mathcal{S}(s)} = \mathcal{K}(s) + [i\mathcal{S}(s), \mathcal{K}(s)]$$

$$+ \frac{1}{2!}[i\mathcal{S}(s), [i\mathcal{S}(s), \mathcal{K}(s)]] + \cdots . \quad (A2)$$

The first commutator can be written as

$$[i\mathcal{S}(s), \mathcal{K}(s)] = -\sum_{m\neq 0} P_m \otimes H_s^{(m)}(s)$$

$$+ \sum_{m\neq 0} \left(\frac{P_m}{m} \otimes \sum_{i=0}^{+\infty} \frac{\left[H_s^{(m)}(s), H_i^{(0)}(s) \right]}{\hbar\omega} \right)$$

$$+ P_0 \otimes \sum_{m\neq 0} \sum_{i=s}^{+\infty} \frac{\left[H_s^{(m)}(s), H_i^{(-m)}(s) \right]}{m\hbar\omega}$$

$$+ \sum_{m\neq 0} \sum_{k\neq\{0,m\}} P_k \otimes \sum_{i=s}^{+\infty} \frac{\left[H_s^{(m)}(s), H_i^{(k-m)}(s) \right]}{m\hbar\omega}.$$

$$(A3)$$

Now we need to consider separately two cases: $s = 0$ and $s \geqslant 1$. For $s \geqslant 1$, we may drop the two last terms from Eq. (A3):

$$[i\mathcal{S}(s), \mathcal{K}(s)] = -\sum_{m \neq 0} P_m \otimes H_s^{(m)}(s)$$
$$+ \sum_{m \neq 0} P_m \otimes \frac{\left[H_s^{(m)}(s), H_0^{(0)}(s)\right]}{m\hbar\omega}$$
$$+ O\left(\frac{1}{(\hbar\omega)^{s+2}}\right). \qquad (A4)$$

The leading term here is the first term on the right-hand side; when added to the Kamiltonian, it will eliminate the sth $-$ order term of the $m \neq 0$ Fourier components that appear in the block off-diagonal part. The double commutator $[i\mathcal{S}, [i\mathcal{S}, \mathcal{K}]]$ and subsequent nested commutators in Eq. (A2) contribute to orders higher than $s + 1$ and need not be considered. The second term on the right-hand side of Eq. (38)

reads

$$-i\hbar e^{i\mathcal{S}(s)} \frac{de^{-i\mathcal{S}(s)}}{dt} = i\hbar[i\dot{\mathcal{S}}(s)] + \frac{i\hbar}{2!}[i\mathcal{S}(s), i\dot{\mathcal{S}}(s)] + \cdots$$
$$= i\hbar \sum_{m \neq 0} P_m \otimes \frac{\dot{H}_s^{(m)}(s)}{m\hbar\omega} + O\left(\frac{1}{(\hbar\omega)^{s+2}}\right). \qquad (A5)$$

Summarizing Eqs. (A2), (A4), and (A5), one can write recursion expressions for the transformed Kamiltonian $\mathcal{K}(s + 1)$. The Fourier components read $H_i^{(m \neq 0)}(s + 1) = 0$ for $i \in [0, s]$ and

$$H_{s+1}^{(m \neq 0)}(s + 1) = H_{s+1}^{(m)}(s) + \frac{\left[H_s^{(m)}(s), H_0^{(0)}(s)\right]}{m\hbar\omega} + \frac{i\dot{H}_s^{(m)}(s)}{m\omega}. \qquad (A6)$$

The relevant contributions to the zeroth Fourier component remain unchanged, $H_i^{(0)}(s + 1) = H_i^{(0)}(s)$ for $i \in [0, s + 1]$.

Proceeding to the case $s = 0$, one should repeat the corresponding analysis starting from Eq. (A3). The analog of Eq. (A4) reads

$$[i\mathcal{S}(0), \mathcal{K}(0)] = -\sum_{m \neq 0} P_m \otimes H_0^{(m)}(0) + \sum_{m \neq 0} P_m \otimes \frac{\left[H_0^{(m)}(0), H_0^{(0)}(0)\right]}{\hbar\omega}$$
$$+ P_0 \otimes \sum_{m \neq 0} \frac{\left[H_0^{(m)}(0), H_0^{(-m)}(0)\right]}{m\hbar\omega} + \sum_{m \neq 0} \sum_{k \neq \{0,m\}} P_k \otimes \frac{\left[H_0^{(m)}(0), H_0^{(k-m)}(0)\right]}{m\hbar\omega} + O\left(\frac{1}{(\hbar\omega)^2}\right). \qquad (A7)$$

Now also the double commutator from Eq. (A2) has to be taken into account:

$$\frac{[i\mathcal{S}(s), [i\mathcal{S}(s), \mathcal{K}(s)]]}{2!} = -P_0 \otimes \sum_{m \neq 0} \frac{\left[H_0^{(m)}(0), H_0^{(-m)}(0)\right]}{2m\hbar\omega}$$
$$- \sum_{m \neq 0} \sum_{k \neq \{0,m\}} P_k \otimes \frac{\left[H_0^{(m)}(0), H_0^{(k-m)}(0)\right]}{2m\hbar\omega} + O\left(\frac{1}{(\hbar\omega)^2}\right). \qquad (A8)$$

Thus the recursive expressions for the $m \neq 0$ Fourier components read $H_0^{(m \neq 0)}(1) = 0$ and

$$H_1^{(m \neq 0)}(1) = H_1^{(m)}(0) + \frac{\left[H_0^{(m)}(0), H_0^{(0)}(0)\right]}{m\hbar\omega} + \sum_{k \neq \{0,m\}} \frac{\left[H_0^{(k)}(0), H_0^{(m-k)}(0)\right]}{2k\hbar\omega} + \frac{i\dot{H}_0^{(m)}(0)}{m\omega}, \qquad (A9)$$

while for the zeroth Fourier component we have $H_0^{(0)}(1) = H_0^{(0)}(0)$ and

$$H_1^{(0)}(1) = H_1^{(0)}(1) + \sum_{m \neq 0} \frac{\left[H_0^{(m)}(0), H_0^{(-m)}(0)\right]}{2m\hbar\omega}. \qquad (A10)$$

Equations (A9) and (A10) can be simplified by taking into account that $H_1^{(m)}(0) = 0$ and $H_0^{(m)}(0) = h^{(m)}$; thus in terms of the Fourier components of the driven Hamiltonian

$$H_1^{(m \neq 0)}(1) = \frac{[h^{(m)}, h^{(0)}]}{m\hbar\omega} + \sum_{k \neq \{0,m\}} \frac{[h^{(k)}, h^{(m-k)}]}{2k\hbar\omega} + \frac{i\dot{h}^{(m)}}{m\omega} \qquad (A11)$$

and

$$H_1^{(0)}(1) = \sum_{m \neq 0} \frac{[h^{(m)}, h^{(-m)}]}{2m\hbar\omega}. \qquad (A12)$$

Now let us return to the case $s \geqslant 1$. By looking at Eqs. (A4) and (A5), one can see that at the flow step $s \to s + 1$ the diagonal Fourier components $H_i^{(0)}$ are not affected for $i \in [0, s + 1]$. Then one can ask at which lowest order the diagonal Fourier components are affected. From the third term of Eq. (A3) one can see that the diagonal Fourier component is modified only with terms proportional to $(\hbar\omega)^{-(2s+1)}$. This means that having obtained the Kamiltonian $K(s)$, we can claim that its diagonal blocks have converged up to the order $2s$, because further steps of the flow will not modify these terms. The upshot of the argument is that from the Kamilto-

nian $K(s)$ we can extract the FE Hamiltonian as

$$h_{\text{eff}} = \sum_{i=0}^{2s} H_i^{(0)}(s) + O\left(\frac{1}{(\hbar\omega)^{2s+1}}\right), \qquad \text{(A13)}$$

that is, the accuracy is much better than anticipated from Eq. (45).

APPENDIX B: SOLUTION OF THE FLOW EQUATIONS (51) IN TERMS OF HIGH-FREQUENCY EXPANSION

In this Appendix we solve Eq. (51) in terms of power series in the inverse frequency. We thus assume that the amplitude of the Fourier components $h^{(m)}(t)$ and their time derivatives $d^j h^{(m)}(t)/dt^j$ are $O(1)$. For the sake of simplicity, in this Appendix we will not write the explicit dependence on time, but will keep it in mind. Each running Fourier component $H^{(m)}(s, t)$ is expanded as

$$H^{(m)}(s) = H_0^{(m)}(s) + H_1^{(m)}(s) + H_2^{(m)}(s) + \cdots, \qquad \text{(B1)}$$

where the expansion terms $H_j^{(m)}(s) \sim O(1/(\hbar\omega)^j)$. The initial conditions are

$$H_0^{(m)}(0) = h^{(m)}, \qquad \text{(B2)}$$

while for any $j \geqslant 1$ we have

$$H_j^{(m)}(0) = 0. \qquad \text{(B3)}$$

Substituting Eq. (B1) into the left- and right-hand sides of Eq. (51), we obtain the zeroth-order flow equations

$$\frac{dH_0^{(0)}(s)}{ds} = 0, \qquad \frac{dH_0^{(n)}(s)}{ds} = -n^2 H_0^{(n)}(s). \qquad \text{(B4)}$$

The solutions to these equations are

$$H_0^{(0)}(s) = h^{(0)}, \qquad H_0^{(n)}(s) = h^{(n)} e^{-n^2 s}. \qquad \text{(B5)}$$

Here we can see that in the limit $s \to +\infty$ the off-diagonal Fourier components vanish, while the diagonal Fourier com-

ponent gives the zeroth-order approximation of the FE Hamiltonian $h_{\text{eff}(0)} = h^{(0)}$.

In the first order, Eq. (51a) gives

$$\frac{dH_1^{(0)}(s)}{ds} = \frac{2}{\hbar\omega} \sum_{m=1}^{+\infty} m[h^{(m)}, h^{(-m)}] e^{-2m^2 s}. \qquad \text{(B6)}$$

By taking into account Eq. (B3), the solution to Eq. (B6) reads

$$H_1^{(0)}(s) = \sum_{m=1}^{+\infty} \frac{[h^{(m)}, h^{(-m)}]}{m\hbar\omega}\left(1 - e^{-2m^2 s}\right). \qquad \text{(B7)}$$

Taking the limit $s \to \infty$, one obtains the first-order approximation of the FE Hamiltonian

$$h_{\text{eff}(1)} = \lim_{s\to+\infty} H_1^{(0)}(s) = \sum_{m=1}^{+\infty} \frac{[h^{(m)}, h^{(-m)}]}{m\hbar\omega}. \qquad \text{(B8)}$$

In the first order Eq. (51b) gives the linear inhomogeneous differential equation

$$\frac{dH_1^{(n)}(s)}{ds} = -n^2 H_1^{(n)}(s) + \frac{in}{\omega}\dot{h}^{(n)} e^{-n^2 s} + \sum_{m\neq n} \frac{m-n}{\hbar\omega}[h^{(m)}, h^{(n-m)}] e^{-[m^2+(n-m)^2]s}. \qquad \text{(B9)}$$

The solution to Eq. (B9) corresponding to the initial conditions (B3) reads

$$H_1^{(n)}(s) = n\left(\frac{i}{\omega}\dot{h}^{(n)} - \frac{[h^{(0)}, h^{(n)}]}{\hbar\omega}\right)se^{-n^2 s} + \sum_{m\neq\{0,n\}} \frac{[h^{(m)}, h^{(n-m)}]}{2m\hbar\omega}\left(e^{-n^2 s} - e^{-[m^2+(n-m)^2]s}\right). \qquad \text{(B10)}$$

One can see that in the limit $s \to +\infty$ the term $H_1^{(n)}(s)$ vanishes.

To proceed further, we collect the second-order terms of Eq. (51a),

$$\frac{dH_2^{(0)}(s)}{ds} = \sum_{n=1}^{+\infty} \frac{2n}{\hbar\omega}\left\{\left[H_1^{(n)}(s), H_0^{(-n)}(s)\right] + \left[H_0^{(n)}(s), H_1^{(-n)}(s)\right]\right\} = \sum_{n\neq 0} \frac{[h^{(n)}, [h^{(0)}, h^{(-n)}]]}{(\hbar\omega)^2} 2n^2 s e^{-2n^2 s}$$

$$+ \sum_{n\neq 0}\sum_{m\neq\{0,n\}} \frac{[h^{(-n)}, [h^{(n-m)}, h^{(m)}]]}{(\hbar\omega)^2}\frac{n}{m}\left(e^{-2n^2 s} - e^{-[m^2+n^2+(n-m)^2]s}\right) + 2i\hbar\sum_{n\neq 0} \frac{[\dot{h}^{(n)}, h^{(-n)}]}{(\hbar\omega)^2} n^2 s e^{-2n^2 s}. \qquad \text{(B11)}$$

The solution corresponding to the initial conditions (B3) reads

$$H_2^{(0)}(s) = \sum_{n\neq 0} \frac{[h^{(n)}, [h^{(0)}, h^{(-n)}]]}{(\hbar\omega)^2}\frac{1 - e^{-2n^2 s}(2n^2 s + 1)}{2n^2}$$

$$+ \sum_{n\neq 0}\sum_{m\neq\{0,n\}} \frac{[h^{(-n)}, [h^{(n-m)}, h^{(m)}]]}{(\hbar\omega)^2}\left\{\frac{1 - e^{-2n^2 s}}{2nm} - \frac{n\left(1 - e^{-[m^2+n^2+(n-m)^2]s}\right)}{m[m^2 + n^2 + (n-m)^2]}\right\}$$

$$+ i\hbar\sum_{n\neq 0} \frac{[\dot{h}^{(n)}, h^{(-n)}]}{(\hbar\omega)^2}\frac{1 - e^{-2n^2 s}(1 + 2n^2 s)}{2n^2}. \qquad \text{(B12)}$$

Taking the limit, one obtains the second-order approximation of the FE Hamiltonian

$$h_{\text{eff}(2)} = \lim_{s \to +\infty} H_2^{(0)}(s)$$

$$= \frac{1}{(\hbar\omega)^2} \sum_{n \neq 0} \left\{ \frac{[h^{(n)}, [h^{(0)}, h^{(-n)}]] + i\hbar[\dot{h}^{(n)}, h^{(-n)}]}{2n^2} + \sum_{m \neq \{0,n\}} \frac{[h^{(-n)}, [h^{(n-m)}, h^{(m)}]](m-n)}{n[m^2 + n^2 + (n-m)^2]} \right\}. \quad (B13)$$

Comparing the obtained results with those given in Ref. [40], one does not immediately appreciate their equivalence. Indeed, the third term of Eq. (B13) reads

$$A = \sum_{n \neq 0} \sum_{m \neq \{0,n\}} [h^{(-n)}, [h^{(n-m)}, h^{(m)}]] f(n, m), \quad (B14)$$

with $f(n, m) = (m - n)/n[m^2 + n^2 + (n - m)^2]$, while the corresponding term from Ref. [40] reads

$$B = \sum_{n \neq 0} \sum_{m \neq \{0,n\}} [h^{(-n)}, [h^{(n-m)}, h^{(m)}]] g(n, m), \quad (B15)$$

with $g(n, m) = 1/3nm$. In Appendix D we show that $A = B$; thus up to the second order the FE Hamiltonian obtained from the flow Eqs. (51) coincides with the results in Ref. [40] as well as in Refs. [33,34].

APPENDIX C: MICROMOTION OPERATOR OBTAINED FROM THE FLOW EQUATIONS (51) IN TERMS OF HIGH-FREQUENCY EXPANSION

In this Appendix we will find the micromotion operator (25) in the exponential form $U_{\text{micro}} = \exp(-iS)$, where the Hermitian operator $S = S_0 + S_1 + S_2 + \cdots$ is obtained as a series expansion with respect to the inverse frequency. With respect to Eq. (43), the extended-space unitary transformation $\mathcal{D}^\dagger(t)$ can be obtained with the help of the Magnus expansion in the exponential form $\mathcal{D}^\dagger(t) = \exp[i(\mathcal{S}_0 + \mathcal{S}_1 + \mathcal{S}_2 + \cdots)]$, where the exponent is expanded in power series with respect to the inverse frequency. The relation between the physical-space operator S_j and the extended-space operator $\mathcal{S}_j = \sum_m P_m \otimes S_j^{(m)}$ is established by simply replacing the shift operator P_m by the exponent $e^{im(\omega t + \theta)}$: $S_j(\omega t + \theta, t) = \sum_m S_j^{(m)}(t) e^{im(\omega t + \theta)}$. In terms of the generator $i\mathcal{S}(s)$, the logarithm of the operator $\mathcal{D}^\dagger$ reads (for the simplicity, in this Appendix we will not write the explicit dependence on time, but will keep it in mind)

$$i(\mathcal{S}_0 + \mathcal{S}_1 + \mathcal{S}_2 + \cdots)$$

$$= \int_0^{+\infty} i\mathcal{S}(s_1) ds_1 + \frac{1}{2} \int_0^{+\infty} \int_0^{s_1} [i\mathcal{S}(s_1), i\mathcal{S}(s_2)]$$

$$\times ds_2 ds_1 + \cdots, \quad (C1)$$

where the generator reads

$$i\mathcal{S}(s) = \sum_{m \neq 0} \frac{m}{\hbar\omega} P_m \otimes H^{(m)}(s). \quad (C2)$$

Note that Eq. (50) differs from the obtained expression (C2) because, similarly to Eq. (51), here we use the rescaled flow variable $s \to s/(\hbar\omega)^2$. Since the expansion of the Fourier components $H^{(m)}(s) = H_0^{(m)}(s) + H_1^{(m)}(s) +$

$H_2^{(m)}(s) + \cdots$ was found analytically in Appendix B, we can derive the analytical expressions for $\mathcal{S}_0$, $\mathcal{S}_1$, and $\mathcal{S}_2$. Let us substitute Eq. (C2) into the right-hand side of Eq. (C1),

$$\sum_{m \neq 0} \left(\frac{m}{\hbar\omega} P_m \otimes \int_0^{+\infty} H_0^{(m)}(s_1) ds_1 \right)$$

$$+ \sum_{m \neq 0} \left(\frac{m}{\hbar\omega} P_m \otimes \int_0^{+\infty} H_1^{(m)}(s_1) ds_1 \right)$$

$$+ \sum_{m \neq 0} \sum_{n \neq 0} \left(\frac{mn}{2(\hbar\omega)^2} P_{m+n} \otimes \int_0^{+\infty} \right.$$

$$\times \left. \int_0^{s_1} \left[H_0^{(m)}(s_1), H_0^{(n)}(s_2) \right] ds_2 ds_1 \right) + \cdots. \quad (C3)$$

This shows that $\mathcal{S}_0 = 0$. Using Eq. (B5) we get

$$\mathcal{S}_1 = \frac{1}{i\hbar\omega} \sum_{m \neq 0} \frac{P_m}{m} \otimes h^{(m)}. \quad (C4)$$

In order to obtain $\mathcal{S}_2$, let us first calculate the double commutator

$$\int_0^{+\infty} \int_0^{s_1} \left[H_0^{(m)}(s_1), H_0^{(n)}(s_2) \right] ds_2 ds_1$$

$$= [h^{(m)}, h^{(n)}] \int_0^{+\infty} e^{-m^2 s_1} \int_0^{s_1} e^{-n^2 s_2} ds_2 ds_1$$

$$= [h^{(m)}, h^{(n)}] \left(\frac{1}{m^2 n^2} - \frac{1}{n^2(m^2 + n^2)} \right). \quad (C5)$$

Next, by using Eq. (B10), we evaluate the integral

$$\int_0^{+\infty} H_1^{(m)}(s_1) ds_1 = \frac{i}{\omega m^3} \dot{h}^{(m)} - \frac{[h^{(0)}, h^{(m)}]}{m^3 \hbar\omega}$$

$$+ \sum_{n \neq \{0,m\}} \frac{[h^{(n)}, h^{(m-n)}]}{2n\hbar\omega}$$

$$\times \left(\frac{1}{m^2} - \frac{1}{n^2 + (m-n)^2} \right). \quad (C6)$$

Now one can collect the second and third terms of Eq. (C3),

$$\mathcal{S}_2 = \frac{1}{2i(\hbar\omega)^2} \sum_{m \neq 0} P_m \otimes \left[2\frac{i\hbar\dot{h}^{(m)}}{m^2} + 2\frac{[h^{(m)}, h^{(0)}]}{m^2} \right.$$

$$+ \sum_{n \neq \{0,m\}} [h^{(n)}, h^{(m-n)}] \left(\frac{1}{nm} - \frac{1}{(m-n)^2 + n^2} \right) \right]$$

$$+ \frac{i}{4(\hbar\omega)^2} P_0 \otimes \sum_{m \neq 0} \frac{[h^{(m)}, h^{(-m)}]}{m^2}. \quad (C7)$$

The obtained result can be simplified. The term proportional to P_0 is zero because any positive-m term will be compensated by a corresponding negative-m term. Another simplification results from the fact that

$$A = \sum_{m \neq 0} \sum_{n \neq \{0,m\}} P_m \otimes \frac{[h^{(n)}, h^{(m-n)}]}{(m-n)^2 + n^2} \qquad \text{(C8)}$$

is equal to zero. Indeed, by applying the transformation of the second variable $n = m - n'$ we get

$$A = -\sum_{m \neq 0} \sum_{n' \neq \{0,m\}} P_m \otimes \frac{[h^{(n')}, h^{(m-n')}]}{(m-n')^2 + n'^2}, \qquad \text{(C9)}$$

which shows that $A = -A$, and thus $A = 0$. Therefore, Eq. (C7) is simplified to

$$S_2 = \frac{1}{2i(\hbar\omega)^2} \sum_{m \neq 0} P_m \otimes \left[2\frac{i\hbar}{m^2} \dot{h}^{(m)} + \frac{[h^{(m)}, h^{(0)}]}{m^2} \right.$$
$$\left. + \sum_{n \neq 0} \frac{[h^{(n)}, h^{(m-n)}]}{nm} \right]. \qquad \text{(C10)}$$

Comparing (C4) and (C10) with the micromotion operator obtained in Ref. [40], we conclude that they coincide.

APPENDIX D: PROOF THAT TWO QUANTITIES (B14) AND (B15) ARE EQUAL

Let us verify that the quantities (B14) and (B15) are equal. The expression (B14) reads

$$A = \sum_{n \neq 0} \sum_{m \neq \{0,n\}} [h^{(-n)}, [h^{(n-m)}, h^{(m)}]] f(n, m), \qquad \text{(D1)}$$

whereas the expression (B15) is of the same form but in place of $f(n, m)$ features a different function $g(n, m)$. Such an ambiguity arises because the summation over the specified values n and m contributes the same commutators from different terms. For example, a simple inspection shows that, for $n = 1$, terms with $m = -1$ and $m = 2$ contribute to the same commutator $[h^{(-1)}, [h^{(2)}, h^{(-1)}]]$. In fact, the same commutator is produced two more times from the remaining terms of the double sum.

To rectify the situation, let us now show that Eq. (D1) can be written in an unambiguous way in terms of commutators of the form $[h^{(-j)}, [h^{(j+\ell)}, h^{(-\ell)}]]$ and $[h^{(j)}, [h^{(-j-\ell)}, h^{(j)}]]$ with positive j and ℓ. In other words, all commutators are thus cast into a standard form where a positive-indexed Fourier component is flanked by two negatived-indexed ones or vice versa. Note that the Fourier indices of all three components participating in a triple commutator sum to zero and zero indices are excluded. Thus one always has two negative indices and a positive one or the other way around. As we will show shortly, the desired transformation is achieved by (i) exchanging the order of the two Fourier components in the inner commutator and (ii) applying the Jacobi identity.

Let us start by observing that the summation $\sum_{n \neq 0} \sum_{m \neq \{0,n\}}$ covers six sectors:

(i) $m < 0 < n$,   (iv) $m < n < 0$,

(ii) $0 < m < n$,   (v) $n < m < 0$,

(iii) $0 < n < m$,   (vi) $n < 0 < m$.

Listed in the left (right) column are the three cases that correspond to the three possible ways to locate m relative to zero and positive (negative) n.

Case (i) is immediately in the form that we want. We relabel $n = j$ and $m = -\ell$ and write

$$\sum_{n>0} \sum_{m<0} [h^{(-n)}, [h^{(n-m)}, h^{(m)}]] f(n, m)$$
$$= \sum_{j>0} \sum_{\ell>0} [h^{(-j)}, [h^{(j+\ell)}, h^{(-\ell)}]] f(j, -\ell). \qquad \text{(D2)}$$

Case (iii) is one that requires the inversion of the order of operators in the inner commutator. We relabel $n = j$ and $m = j + \ell$ and obtain

$$\sum_{n>0} \sum_{m>n} [h^{(-n)}, [h^{(n-m)}, h^{(m)}]] f(n, m)$$
$$= -\sum_{j>0} \sum_{\ell>0} [h^{(-j)}, [h^{(j+\ell)}, h^{(-\ell)}]] f(j, j+\ell). \qquad \text{(D3)}$$

Finally, case (v) is one that requires the application of the Jacobi identity and subsequent inversion of the inner commutator in one of the two resulting terms. Carrying out the algebra and introducing positive indices j and ℓ as above, we find

$$\sum_{m<0} \sum_{n<m} [h^{(-n)}, [h^{(n-m)}, h^{(m)}]] f(n, m)$$
$$= \sum_{j>0} \sum_{\ell>0} [h^{(-j)}, [h^{(j+\ell)}, h^{(-\ell)}]] f(-j-\ell, -\ell)$$
$$- \sum_{j>0} \sum_{\ell>0} [h^{(-j)}, [h^{(j+\ell)}, h^{(-\ell)}]] f(-j-\ell, -j). \qquad \text{(D4)}$$

The considered cases (i), (iii), and (v) cover the terms that lead to a positive-indexed Fourier component flanked by two negative-indexed ones. All in all, they sum up to the final result

$$\sum_{m<0} \sum_{n<m} [h^{(-n)}, [h^{(n-m)}, h^{(m)}]] f(n, m)$$
$$= \sum_{j>0} \sum_{\ell>0} [h^{(-j)}, [h^{(j+\ell)}, h^{(-\ell)}]] \tilde{f}(j, \ell), \qquad \text{(D5)}$$

with

$$\tilde{f}(j, \ell) = f(j, -\ell) - f(j, j+\ell)$$
$$+ f(-j-\ell, -\ell) - f(-j-\ell, -j). \qquad \text{(D6)}$$

Using

$$f(n, m) = \frac{m-n}{n[n^2 + m^2 + (m-n)^2]}, \qquad \text{(D7)}$$

we find

$$\tilde{f}(j, \ell) = \frac{-1}{j(j+\ell)}, \qquad \text{(D8)}$$

and using

$$g(n, m) = \frac{1}{3nm}, \qquad \text{(D9)}$$

we find

$$\tilde{g}(j, \ell) = \frac{-1}{j(j + \ell)}. \tag{D10}$$

The consideration of cases (ii), (iv), and (vi) is identical in spirit and restructures the complementary case where a single negative-indexed Fourier component is flanked by two positive-indexed ones.

APPENDIX E: TODA FLOW EQUATIONS FOR THE CASE OF A LIMITED NUMBER OF HARMONICS

In this Appendix we prove the statement made in the main text: If the initial condition for Eq. (53b) has a limited number of nonvanishing Fourier harmonics at $s = 0$, i.e., $H^{(n)}(0, t) = 0$ for all $|n| > n_0$, then these high harmonics (with $|n| > n_0$) may be neglected altogether since they will not be populated in the course of the flow. This implies that the flow needs to be analyzed only for the limited spectrum with harmonics $|n| \leqslant n_0$. For notational simplicity, we will not write the explicit dependence on time, but will keep it in mind.

Let us first rewrite Eq. (53b) as

$$\frac{dH^{(n)}(s)}{ds} = -n \operatorname{sgn}(n) H^{(n)}(s) + \frac{i}{\omega} \operatorname{sgn}(n) \dot{H}^{(n)}(s)$$
$$- \frac{\operatorname{sgn}(n)}{\hbar \omega} [H^{(0)}(s), H^{(n)}(s)]$$
$$+ \sum_{m \neq \{0, n\}} \frac{\operatorname{sgn}(m - n)}{\hbar \omega} [H^{(m)}(s), H^{(n-m)}(s)] \tag{E1}$$

and focus on the last term of Eq. (E1). We distinguish two cases: when n is odd and when n is even. In both cases, instead of m we introduce new index $l = 2m - n$. For an odd n we have $l = \{\pm 1, \pm 3, \dots\}$, whereas for even n the permissible values of l read $l = \{0, \pm 2, \pm 4, \dots\}$. From the condition $m \neq \{0, n\}$ we obtain $l \neq \pm n$. Thus, for the case of an odd value of n the term in question reads

$$\sum_{l = \{\pm 1, \pm 3, \dots, \neq \pm n, \dots\}} \operatorname{sgn}\left(\frac{l - n}{2}\right) [H^{((n+l)/2)}(s), H^{((n-l)/2)}(s)]. \tag{E2}$$

The denominator 2 in the argument of the sign function $\operatorname{sgn}(\cdot)$ can be omitted. We split Eq. (E2) into two terms separating positive and negative values of l and introduce the replace-

ment $l' = -l$ for the negative l's with the result

$$\sum_{l' = \{1, 3, \dots, \neq |n|, \dots\}} \operatorname{sgn}(-l' - n) [H^{((n-l')/2)}(s), H^{((n+l')/2)}(s)]$$
$$= \sum_{l' = \{1, 3, \dots, \neq |n|, \dots\}} \operatorname{sgn}(l' + n) [H^{((n+l')/2)}(s), H^{((n-l')/2)}(s)]. \tag{E3}$$

We now sum the obtained expression with its counterpart for positive values of l and obtain

$$\sum_{l = \{1, 3, \dots, \neq |n|, \dots\}} \{\operatorname{sgn}(n + l) - \operatorname{sgn}(n - l)\}$$
$$\times [H^{((n+l)/2)}(s), H^{((n-l)/2)}(s)]. \tag{E4}$$

Let us now consider the combination of sign functions in the curly braces. For $l < |n|$ the expression in the braces yields zero: If n is positive, then $n + l > 0$ and $n - l > 0$; if n is negative then $n + l < 0$ and $n - l < 0$. On the other hand, for $l > |n|$ the terms in parentheses are equal to 2. Thus, the expression in Eq. (E4) can be simplified to

$$2 \sum_{l = \{|n|+2, |n|+4, \dots\}} [H^{((n+l)/2)}(s), H^{((n-l)/2)}(s)]. \tag{E5}$$

By performing a similar procedure that led from Eq. (E2) to Eq. (E5) for the case of n even, one arrives at the same expression (E5). Therefore, Eq. (E1) transforms to

$$\frac{dH^{(n)}(s)}{ds} = -n \operatorname{sgn}(n) H^{(n)}(s) + \frac{i}{\omega} \operatorname{sgn}(n) \dot{H}^{(n)}(s)$$
$$- \frac{\operatorname{sgn}(n)}{\hbar \omega} [H^{(0)}(s), H^{(n)}(s)]$$
$$+ \frac{2}{\hbar \omega} \sum_{l = \{|n|+2, |n|+4, \dots\}} [H^{((n+l)/2)}(s), H^{((n-l)/2)}(s)]. \tag{E6}$$

From Eq. (E6) one can see that if $n > |n_0|$, even with smallest possible $l = |n| + 2$, one of the indices of the Fourier harmonics $(n + l)/2 = (n + |n|)/2 + 1$ and $(n - l)/2 = (n - |n|)/2 - 1$ will have an absolute value higher than n_0, and thus the commutator will vanish. All the other terms on the right-hand side of Eq. (E6) also vanish for $n > |n_0|$.

For harmonics with small indices $n \leqslant |n_0|$, the index l in Eq. (E6) can be restricted to $l = \{|n| + 2, |n| + 4, \dots, |n| + 2(n_0 - |n|)\}$. Finally, Eq. (E6) reads [here we rename the index $l \rightarrow (l - |n|)/2$]

$$\frac{dH^{(n)}(s)}{ds} = \begin{cases} -nH^{(n)}(s) + \frac{i}{\omega}\dot{H}^{(n)}(s) + \frac{[H^{(n)}(s), H^{(0)}(s)]}{\hbar\omega} + \frac{2}{\hbar\omega}\sum_{l=1}^{n_0-n}[H^{(n+l)}(s), H^{(-l)}(s)] & \text{for } 0 < n \leqslant n_0 \\ nH^{(n)}(s) - \frac{i}{\omega}\dot{H}^{(n)}(s) + \frac{[H^{(0)}(s), H^{(n)}(s)]}{\hbar\omega} + \frac{2}{\hbar\omega}\sum_{l=1}^{n_0+n}[H^{(l)}(s), H^{(n-l)}(s)] & \text{for } -n_0 \leqslant n < 0 \\ 0 & \text{for } |n| > n_0. \end{cases} \tag{E7}$$

The flow equation for the zeroth Fourier harmonic reads

$$\frac{dH^{(0)}(s)}{ds} = \frac{2}{\hbar \omega} \sum_{m=1}^{n_0} [H^{(m)}(s), H^{(-m)}(s)]. \tag{E8}$$

APPENDIX F: AUTOMATED EXPANSION OF THE FE HAMILTONIAN AND MICROMOTION OPERATOR FOR THE RABI LINEARLY POLARIZED DRIVE

We perform the automated solution of the flow Eqs. (53) with the initial conditions (58). For $\phi = 0$, the effective Hamiltonian reads ($\hbar = 1$)

$$h_{\text{eff}} = \sigma_x \left[g(t) - \frac{g(t)^3}{4\omega^2} + \frac{3\Delta g(t)^3}{16\omega^3} + \frac{-6g(t)g'(t)^2 + 7g(t)^2 g''(t) - 7\Delta^2 g(t)^3 - 8g(t)^5}{64\omega^4} \right] + \sigma_y \left[-\frac{g(t)^2 g'(t)}{16\omega^3} + \frac{\Delta g(t)^2 g'(t)}{16\omega^4} \right]$$

$$+ \sigma_z \left[\frac{\Delta}{2} + \frac{g(t)^2}{2\omega} + -\frac{\Delta g(t)^2}{4\omega^2} \frac{g'(t)^2 - g(t)g''(t) + 2\Delta^2 g(t)^2}{16\omega^3} + \frac{-3\Delta g'(t)^2 + 3\Delta g(t)g''(t) - 2\Delta^3 g(t)^2 + \Delta g(t)^4}{32\omega^4} \right]. \quad \text{(F1)}$$

Higher-order contributions were obtained (also in the general case $\phi \neq 0$) but are not suitable for reproduction on a journal page. The MATHEMATICA script used to generate expansions up to the fifth order is available from [72].

[1] P. Hänggi, in *Quantum Transport and Dissipation*, edited by T. Dittrich, P. Hänggi, G.-L. Ingold, B. Kramer, G. Schön, and W. Zwerger (Wiley-VCH, Weinheim, 1998), Chap. 5, pp. 249–286.

[2] M. Holthaus, Floquet engineering with quasienergy bands of periodically driven optical lattices, J. Phys. B **49**, 013001 (2016).

[3] A. Eckardt, Colloquium: Atomic quantum gases in periodically driven optical lattices, Rev. Mod. Phys. **89**, 011004 (2017).

[4] J. S. Howland, Stationary scattering theory for time-dependent Hamiltonians, Math. Ann. **207**, 315 (1974).

[5] U. Peskin and N. Moiseyev, The solution of the time-dependent Schrödinger equation by the (t, t') method: Theory, computational algorithm and applications, J. Chem. Phys. **99**, 4590 (1993).

[6] P.-L. Giscard and C. Bonhomme, Dynamics of quantum systems driven by time-varying Hamiltonians: Solution for the Bloch-Siegert Hamiltonian and applications to NMR, Phys. Rev. Research **2**, 023081 (2020).

[7] J. H. Shirley, Solution of the Schrödinger equation with a Hamiltonian periodic in time, Phys. Rev. **138**, B979 (1965).

[8] H. Sambe, Steady states and quasienergies of a quantum-mechanical system in an oscillating field, Phys. Rev. A **7**, 2203 (1973).

[9] F. Casas, J. A. Oteo, and J. Ros, Floquet theory: Exponential perturbative treatment, J. Phys. A: Math. Gen. **34**, 3379 (2001).

[10] T. Oka and H. Aoki, Photovoltaic Hall effect in graphene, Phys. Rev. B **79**, 081406(R) (2009).

[11] N. H. Lindner, G. Refael, and V. Galitski, Floquet topological insulator in semiconductor quantum wells, Nat. Phys. **7**, 490 (2011).

[12] Z. Gu, H. A. Fertig, D. P. Arovas, and A. Auerbach, Floquet Spectrum and Transport Through an Irradiated Graphene Ribbon, Phys. Rev. Lett. **107**, 216601 (2011).

[13] T. Kitagawa, T. Oka, A. Brataas, L. Fu, and E. Demler, Transport properties of nonequilibrium systems under the application of light: Photoinduced quantum Hall insulators without Landau levels, Phys. Rev. B **84**, 235108 (2011).

[14] M. Bukov, L. D'Alessio, and A. Polkovnikov, Universal high-frequency behavior of periodically driven systems: From dynamical stabilization to Floquet engineering, Adv. Phys. **64**, 139 (2015).

[15] T. Oka and S. Kitamura, Floquet engineering of quantum materials, Annu. Rev. Condens. Matter Phys. **10**, 387 (2019).

[16] M. S. Rudner and N. H. Lindner, Band structure engineering and non-equilibrium dynamics in Floquet topological insulators, Nat. Rev. Phys. **2**, 229 (2020).

[17] U. Bajpai, M. J. H. Ku, and B. K. Nikolić, Robustness of quantized transport through edge states of finite length: Imaging current density in Floquet topological versus quantum spin and anomalous Hall insulators, Phys. Rev. Research **2**, 033438 (2020).

[18] M. Rodriguez-Vega, M. Vogl, and G. A. Fiete, Low-frequency and Moiré-Floquet engineering: A review, Ann. Phys. (NY) **435**, 168434 (2021).

[19] M. Aidelsburger, M. Atala, S. Nascimbène, S. Trotzky, Y.-A. Chen, and I. Bloch, Experimental Realization of Strong Effective Magnetic Fields in an Optical Lattice, Phys. Rev. Lett. **107**, 255301 (2011).

[20] M. Aidelsburger, M. Atala, M. Lohse, J. T. Barreiro, B. Paredes, and I. Bloch, Realization of the Hofstadter Hamiltonian with Ultracold Atoms in Optical Lattices, Phys. Rev. Lett. **111**, 185301 (2013).

[21] J. Struck, M. Weinberg, C. Ölschläger, P. Windpassinger, J. Simonet, K. Sengstock, R. Höppner, P. Hauke, A. Eckardt, M. Lewenstein, and L. Mathey, Engineering Ising-XY spin models in a triangular lattice via tunable artificial gauge fields, Nat. Phys. **9**, 738 (2013).

[22] M. Aidelsburger, M. Lohse, C. Schweizer, M. Atala, J. T. Barreiro, S. Nascimbène, N. R. Cooper, I. Bloch, and N. Goldman, Measuring the Chern number of Hofstadter bands with ultracold bosonic atoms, Nat. Phys. **11**, 162 (2015).

[23] N. Fläschner, B. S. Rem, M. Tarnowski, D. Vogel, D.-S. Lühmann, K. Sengstock, and C. Weitenberg, Experimental reconstruction of the Berry curvature in a Floquet Bloch band, Science **352**, 1091 (2016).

[24] F. Schäfer, T. Fukuhara, S. Sugawa, Y. Takasu, and Y. Takahashi, Tools for quantum simulation with ultracold atoms in optical lattices, Nat. Rev. Phys. **2**, 411 (2020).

[25] J. W. McIver, B. Schulte, F.-U. Stein, T. Matsuyama, G. Jotzu, G. Meier, and A. Cavalleri, Light-induced anomalous Hall effect in graphene, Nat. Phys. **16**, 38 (2020).

[26] T. Kitagawa, E. Berg, M. Rudner, and E. Demler, Topological characterization of periodically driven quantum systems, Phys. Rev. B **82**, 235114 (2010).

[27] J. Cayssol, B. Dóra, F. Simon, and R. Moessner, Floquet topological insulators, Phys. Status Solidi **7**, 101 (2013).

[28] L. E. F. Foa Torres, P. M. Perez-Piskunow, C. A. Balseiro, and G. Usaj, Multiterminal Conductance of a Floquet Topological Insulator, Phys. Rev. Lett. **113**, 266801 (2014).

[29] A. G. Grushin, A. Gómez-León, and T. Neupert, Floquet Fractional Chern Insulators, Phys. Rev. Lett. **112**, 156801 (2014).

[30] A. Farrell and T. Pereg-Barnea, Edge-state transport in Floquet topological insulators, Phys. Rev. B **93**, 045121 (2016).

[31] A. Huamán and G. Usaj, Floquet spectrum and two-terminal conductance of a transition-metal dichalcogenide ribbon under a circularly polarized laser field, Phys. Rev. B **99**, 075423 (2019).

[32] S. Rahav, I. Gilary, and S. Fishman, Effective Hamiltonians for periodically driven systems, Phys. Rev. A **68**, 013820 (2003).

[33] N. Goldman and J. Dalibard, Periodically Driven Quantum Systems: Effective Hamiltonians and Engineered Gauge Fields, Phys. Rev. X **4**, 031027 (2014).

[34] A. Eckardt and E. Anisimovas, High-frequency approximation for periodically driven quantum systems from a Floquet-space perspective, New J. Phys. **17**, 093039 (2015).

[35] E. S. Mananga and T. Charpentier, Introduction of the Floquet-Magnus expansion in solid-state nuclear magnetic resonance spectroscopy, J. Chem. Phys. **135**, 044109 (2011).

[36] E. S. Mananga and T. Charpentier, On the Floquet-Magnus expansion: Applications in solid-state nuclear magnetic resonance and physics, Phys. Rep. **609**, 1 (2016).

[37] A. Verdeny, A. Mielke, and F. Mintert, Accurate Effective Hamiltonians via Unitary Flow in Floquet Space, Phys. Rev. Lett. **111**, 175301 (2013).

[38] T. Mikami, S. Kitamura, K. Yasuda, N. Tsuji, T. Oka, and H. Aoki, Brillouin-Wigner theory for high-frequency expansion in periodically driven systems: Application to Floquet topological insulators, Phys. Rev. B **93**, 144307 (2016).

[39] M. Vogl, P. Laurell, A. D. Barr, and G. A. Fiete, Flow Equation Approach to Periodically Driven Quantum Systems, Phys. Rev. X **9**, 021037 (2019).

[40] V. Novičenko, E. Anisimovas, and G. Juzeliūnas, Floquet analysis of a quantum system with modulated periodic driving, Phys. Rev. A **95**, 023615 (2017).

[41] F. Haddadfarshi, J. Cui, and F. Mintert, Completely Positive Approximate Solutions of Driven Open Quantum Systems, Phys. Rev. Lett. **114**, 130402 (2015).

[42] C. M. Dai, Z. C. Shi, and X. X. Yi, Floquet theorem with open systems and its applications, Phys. Rev. A **93**, 032121 (2016).

[43] S. Restrepo, J. Cerrillo, V. M. Bastidas, D. G. Angelakis, and T. Brandes, Driven Open Quantum Systems and Floquet Stroboscopic Dynamics, Phys. Rev. Lett. **117**, 250401 (2016).

[44] A. Schnell, S. Denisov, and A. Eckardt, High-frequency expansions for time-periodic Lindblad generators, Phys. Rev. B **104**, 165414 (2021).

[45] T. N. Ikeda, K. Chinzei, and M. Sato, Nonequilibrium steady states in the Floquet-Lindblad systems van Vleck's high-frequency expansion approach, SciPost Phys. Core **4**, 033 (2021).

[46] C. M. Dai, H. Li, W. Wang, and X. X. Yi, Generalized Floquet theory for open quantum systems, arXiv:1707.05030.

[47] P. Weinberg, M. Bukov, L. D'Alessio, A. Polkovnikov, S. Vajna, and M. Kolodrubetz, Adiabatic perturbation theory and geometry of periodically-driven systems, Phys. Rep. **688**, 1 (2017).

[48] D. Zeuch, F. Hassler, J. J. Slim, and D. P. DiVincenzo, Exact rotating wave approximation, Ann. Phys. (NY) **423**, 168327 (2020).

[49] D. Zeuch and D. P. DiVincenzo, Refuting a proposed axiom for defining the exact rotating wave approximation, arXiv:2010.02751.

[50] R. Desbuquois, M. Messer, F. Görg, K. Sandholzer, G. Jotzu, and T. Esslinger, Controlling the Floquet state population and observing micromotion in a periodically driven two-body quantum system, Phys. Rev. A **96**, 053602 (2017).

[51] F. Wilczek and A. Zee, Appearance of Gauge Structure in Simple Dynamical Systems, Phys. Rev. Lett. **52**, 2111 (1984).

[52] S. Kehrein, *The Flow Equation Approach to Many-Particle Systems*, Springer Tracts in Modern Physics Vol. 217 (Springer, Berlin, 2006).

[53] C. Tomaras and S. Kehrein, Scaling approach for the time-dependent Kondo model, Europhys. Lett. **93**, 47011 (2011).

[54] C. Monthus, Flow towards diagonalization for many-body-localization models: Adaptation of the Toda matrix differential flow to random quantum spin chains, J. Phys. A: Math. Theor. **49**, 305002 (2016).

[55] S. J. Thomson and M. Schiró, Time evolution of many-body localized systems with the flow equation approach, Phys. Rev. B **97**, 060201(R) (2018).

[56] S. J. Thomson and M. Schiró, Dynamics of disordered quantum systems using flow equations, Eur. Phys. J. B **93**, 22 (2020).

[57] S. P. Kelly, R. Nandkishore, and J. Marino, Exploring many-body localization in quantum systems coupled to an environment via Wegner-Wilson flows, Nucl. Phys. B **951**, 114886 (2020).

[58] F. Wegner, Flow-equations for Hamiltonians, Ann. Phys. (Leipzig) **506**, 77 (1994).

[59] S. D. Głazek and K. G. Wilson, Renormalization of Hamiltonians, Phys. Rev. D **48**, 5863 (1993).

[60] S. D. Glazek and K. G. Wilson, Perturbative renormalization group for Hamiltonians, Phys. Rev. D **49**, 4214 (1994).

[61] W. Magnus, On the exponential solution of differential equations for a linear operator, Commun. Pure Appl. Math. **7**, 649 (1954).

[62] S. Blanes, F. Casas, J. Oteo, and J. Ros, The Magnus expansion and some of its applications, Phys. Rep. **470**, 151 (2009).

[63] S. Guerin and H. R. Jauslin, Control of quantum dynamics by laser pulses: Adiabatic Floquet theory, Adv. Chem. Phys. **125**, 147 (2003).

[64] G. H. Golub and H. A. van der Vorst, Eigenvalue computation in the 20th century, J. Comput. Appl. Math. **123**, 35 (2000), Numerical Analysis 2000. Vol. III: Linear Algebra.

[65] S. R. White, Numerical canonical transformation approach to quantum many-body problems, J. Chem. Phys. **117**, 7472 (2002).

[66] H. Hergert, S. K. Bogner, T. D. Morris, S. Binder, A. Calci, J. Langhammer, and R. Roth, *Ab initio* multireference in-medium similarity renormalization group calculations of even calcium and nickel isotopes, Phys. Rev. C **90**, 041302(R) (2014).

[67] A. Mielke, Flow equations for band-matrices, Eur. Phys. J. B **5**, 605 (1998).

[68] M. Hénon, Integrals of the Toda lattice, Phys. Rev. B **9**, 1921 (1974).

[69] S. Thomson, D. Magano, and M. Schiró, Flow equations for disordered Floquet systems, SciPost Phys. **11**, 028 (2021).

[70] V. Novičenko and G. Juzeliūnas, Non-Abelian geometric phases in periodically driven systems, Phys. Rev. A **100**, 012127 (2019).

[71] E. Anisimovas, G. Žlabys, B. M. Anderson, G. Juzeliūnas, and A. Eckardt, Role of real-space micromotion for bosonic and fermionic Floquet fractional Chern insulators, Phys. Rev. B **91**, 245135 (2015).

[72] http://www.itpa.lt/~novicenko/files/mathematica_scripts/toda_script.nb.